NATIONAL ADVISORY COMMITTEE FOR AERONAUTICS

TECHNICAL NOTE 3154

INFRARED SPECTRA OF 47 DICYCLIC HYDROCARBONS

By John H. Lamneck, Jr., Harold F. Hipsher, and Virginia O. Fenn

Lewis Flight Propulsion Laboratory
Cleveland, Ohio

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SUMMARY

The infrared spectra are presented for 47 dicyclic hydrocarbons consisting of some alkyldiphenylmethanes, alkyldicyclohexylmethanes, alkylnaphthalenes, alkyltetralins, 1,3-diphenyl-2-alkylpropanes and 1,3-dicyclohexyl-2-alkylpropanes. The physical properties of these highly purified compounds are included for reference purposes.

INTRODUCTION

In the course of a study on the effect of structure on the physical properties of dicyclic hydrocarbons, a group of 47 hydrocarbons was synthesized and purified at the NACA Lewis laboratory. This group included twelve alkyldiphenylmethanes, thirteen alkyldicyclohexylmethanes, seven alkylnaphthalenes, nine alkyltetralins, three 1,3-diphenyl-2-alkylpropanes, and three 1,3-dicyclohexyl-2-alkylpropanes. The preparation, purification, and properties of most of these hydrocarbons are reported in references 1 to 6. The remaining compounds are reported in a paper soon to be submitted for publication in the Journal of the American Chemical Society.

Because of the increasing use of infrared spectra in analysis and identification, it was deemed desirable to compile the infrared spectra of these 47 hydrocarbons which were available in a high state of purity. The infrared spectra of 59 dicyclic hydrocarbons were previously published at this laboratory (ref. 7).

MATERIALS

The properties of the alkyldiphenylmethanes are listed in table I. The hydrogenation products of these alkyldiphenylmethanes, the alkyldicyclohexylmethanes, were separated by high-efficiency fractionation into two geometric isomers and are designated in table II as the low- and

high-boiling isomers. The properties of the alkylnaphthalenes are listed in table III. The partial hydrogenation of these naphthalenes yielded the 1- and 5-alkyl-substituted tetralins, but only the 5-isomers could be purified. The 1-substituted isomers were prepared independently (ref. 5). The properties of both alkyltetralin isomers are presented in table IV and the properties of the 1,3-diphenyl- and 1,3-dicyclohexyl-2-alkylpropanes are listed in table V.

The procedures used in evaluating these properties, together with the accuracy and precision of each method, are reported in reference 8. The purities of all of the compounds whose melting points are recorded to 0.01° C have been calculated according to the method of Glasgow, Streiff, and Rossini (ref. 9) to be greater than 99 mole percent. It is not possible to estimate the purity of the other compounds. However, from the methods of purification employed and the analysis of the fractionation data, it is believed that purities of the order of magnitude of 99 mole percent have been obtained.

Each sample was freshly distilled and passed through silica gel just prior to the determination of the infrared spectra.

APPARATUS AND PROCEDURE

The infrared spectra shown in figures 1 to 6 were obtained with a double-beam recording spectrophotometer. The precision of the instrument is specified by the manufacturer to be ±1 percent of the transmission value and ±0.02 microns for the wavelength (ref. 10). In a 0.1-millimeter-thick cell, samples were run both undiluted and, over some wavelength intervals, at approximately 1:10 dilution on a volume basis. The pure solvent was used in the reference beam to nullify the effect of any absorption due to the solvent.

Lewis Flight Propulsion Laboratory
National Advisory Committee for Aeronautics
Cleveland, Ohio, April 29, 1954

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10. Anon.: Infrared Recording Spectrophotometer. Bull. XXX, Baird Associates, Inc. (Cambridge, Mass.).

TABLE I - PROPERTIES OF ALKYLDIPHENYLMETHANE HYDROCARBONS

Hydrocarbon	Melting point, °C	Boiling point at 760 mm, °C	Index of refraction, n_D^{20}	Density at 20° C, g/ml	Kinematic viscosity[a], centistokes				Net heat of combustion, kcal/mole
					98.9° C (210° F)	60° C (140° F)	37.8° C (100° F)	0° C (32° F)	
2-Methyldiphenylmethane	6.61	280.50	1.5763	1.00198	1.18	2.08	3.26	10.81[b]	1735
3-Methyldiphenylmethane	-27.83[c]	279.24	1.5712	.99135	1.07	1.76	2.58	6.84	1750
4-Methyldiphenylmethane	4.58	281.96	1.5692	.98739	1.01	1.61	2.30	5.62[b]	1745
2-Ethyldiphenylmethane	-11.15	290.86	1.5701	.99213	1.23	2.21	3.43	11.20	1880
3-Ethyldiphenylmethane	-9.22	291.54	1.5634	.97976	1.13	1.85	2.71	6.97	1875
4-Ethyldiphenylmethane	-23.52	297.03	1.5630	.97773	1.08	1.75	2.49	6.01	1875
4-Propyldiphenylmethane	-22.48	311.12	1.5556	0.96618	1.29	2.18	3.27	9.01	2025
4-Isopropyldiphenylmethane	-13.36	305.60	1.5554	.96634	1.25	2.08	3.11	8.46	2045
2-Butyldiphenylmethane	-16.56	315.18	1.5536	.96677	1.50	2.83	4.78	20.17	2170
4-Butyldiphenylmethane	-34.95[d]	326.41	1.5492	.95696	1.43	2.43	3.68	10.48	2175
2-sec-Butyldiphenylmethane	-27.52	305.63	1.5545	.96926	1.56	3.10	5.53	30.91	2170
4-sec-Butyldiphenylmethane	-20.86	318.59	1.5500	.95907	1.44	2.53	3.95	12.79	2165

[a]A.S.T.M. procedure: D445-46T.
[b]Supercooled liquid.
[c]A second modification was found to melt at -34.46°.
[d]A second modification was found to melt at -40.62°.

TABLE II - PROPERTIES OF ALKYLDICYCLOHEXYLMETHANE HYDROCARBONS

Hydrocarbon	Melting point, °C	Boiling point at 760 mm, °C	Index of refraction, n_D^{20}	Density at 20° C, g/ml	Kinematic viscosity[a], centistokes				Net heat of combustion, kcal/mole
					98.9° C (210° F)	60° C (140° F)	37.8° C (100° F)	0° C (32° F)	
2-Methyldicyclohexylmethane[b]	-28.06	264.61	1.4760	0.87458	1.42	2.55	3.99	13.11	1975
2-Methyldicyclohexylmethane[c]	-32.5[d]	267.94	1.4799	.88495	1.68	3.20	5.36	21.39	1985
3-Methyldicyclohexylmethane[b]	-38.4[d]	263.25	1.4727	.86713	1.38	2.49	3.99	13.99	1985
3-Methyldicyclohexylmethane[c]	Glass	264.32	1.4756	.87571	1.53	2.84	4.63	17.00	1990
4-Methyldicyclohexylmethane[b]	-25.53	265.07	1.4710	.86410	1.43	2.60	4.16	14.11	2000
4-Methyldicyclohexylmethane[c]	-28.49	266.84	1.4760	.87603	1.62	3.02	4.96	18.07	1990
2-Ethyldicyclohexylmethane[b]	Glass	280.94	1.4796	.88143	1.63	3.10	5.25	23.72	2150
2-Ethyldicyclohexylmethane[c]	-31.2[d]	282.35	1.4813	0.88660	1.70	3.30	5.68	25.93	2135
3-Ethyldicyclohexylmethane[c]	Glass	281.35	1.4746	.87046	1.61	3.09	5.20	21.53	2135
4-Ethyldicyclohexylmethane[b]	-24.93	285.91	1.4731	.86749	1.67	3.18	5.28	20.25	2150
4-Ethyldicyclohexylmethane[c]	Glass	286.15	1.4771	.87774	1.79	3.40	5.67	21.51	2135
4-Isopropyldicyclohexylmethane[b]	Glass	300.22	1.4780	.87839	2.18	4.47	8.04	40.05	2280
4-Isopropyldicyclohexylmethane[c]	Glass	301.81	1.4752	.87082	2.04	4.17	7.47	37.98	2275

[a]A.S.T.M. procedure: D445-46T.
[b]Low-boiling isomer.
[c]High-boiling isomer.
[d]Equilibrium portion of melting curve was very short.

TABLE III - PROPERTIES OF ALKYNAPHTHALENE HYDROCARBONS

Hydrocarbon	Melting point, °C	Boiling point at 760 mm, °C	Index of refraction, n_D^{20}	Density at 20° C, g/ml	Kinematic viscosity[a], centistokes				Net heat of combustion, kcal/mole
					98.9° C (210° F)	60° C (140° F)	37.8° C (100° F)	0° C (32° F)	
1-Methylnaphthalene	-30.50	244.42	1.6174	1.02015	0.92	1.51	2.21	5.99	1345
1-Ethylnaphthalene	-13.88	258.67	1.6062	1.00816	.99	1.68	2.57	7.83	1475
1-Propylnaphthalene	-8.60	272.78	1.5923	.98970	1.11	2.00	3.20	11.48	1630
1-Isopropylnaphthalene	-15.66	267.79	1.5952	.99565	1.11	2.00	3.20	11.88	1630
1-Butylnaphthalene	-19.76	289.34	1.5819	.97673	1.28	2.37	3.95	15.86	1775
1-Isobutylnaphthalene	-9.37[b]	279.54	1.5794	.97144	1.32	2.55	4.42	23.53	1770
1-Amylnaphthalene	-24.54	305.15	1.5726	.96609	1.48	2.86	4.96	22.74	1920

[a]A.S.T.M. procedure: D445-46T.
[b]A second modification was found to melt at -22.14°.

TABLE IV. - PROPERTIES OF ALKYLTETRALIN HYDROCARBONS

Hydrocarbon	Melting point, °C	Boiling point at 760 mm, °C	Index of refraction, n_D^{20}	Density at 20° C, g/ml	Kinematic viscosity[a], centistokes				Net heat of combustion, kcal/mole
					98.9° C (210° F)	60° C (140° F)	37.8° C (100° F)	0° C (32° F)	
1-Methyltetralin	Glass	220.54	1.5353	0.95825	0.88	1.42	2.05	5.08	1425
5-Methyltetralin	-23.05	234.20	1.5440	.97106	.93	1.52	2.22	5.81	1425
1-Ethyltetralin	Glass	239.46	1.5318	.95285	.93	1.54	2.25	6.18	1570
5-Ethyltetralin	-44.55	248.02	1.5398	.96286	.99	1.62	2.40	6.37	1570
1-Butyltetralin	Glass	273.00	1.5218	.93418	1.22	2.20	3.48	12.54	1860
5-Butyltetralin	-49[b]	279.91	1.5280	.94093	1.31	2.40	3.93	14.95	1860
1-Isobutyltetralin	Glass	266.31	1.5198	.93080	1.14	2.01	3.18	11.37	1850
5-Isobutyltetralin	-14.75	270.41	1.5269	.93776	1.34	2.57	4.43	21.80	1860
1-Amyltetralin	Glass	289.49	1.5178	.92705	1.39	2.59	4.30	16.91	2010

[a]A.S.T.M. procedure: D445-46T.
[b]Crystallization unsatisfactory.

TABLE V. - PROPERTIES OF 1,3-DIPHENYL-2-ALKYLPROPANE AND 1,3-DICYCLOHEXYL-2-ALKYLPROPANE HYDROCARBONS

Hydrocarbon	Melting point, °C.	Boiling point[a] at 760 mm, °C	Index of refraction, n_D^{20}	Density at 20° C, g/ml	Kinematic viscosity,[b] centistokes				Net heat of combustion, kcal/mole
					98.9° C (210° F)	60° C (140° F)	37.8° C (100° F)	0° C (32° F)	
1,3-Diphenyl-2-methylpropane	-33.7[c]	303.0	1.5519	0.96694	31.8	5.44	3.03	1.51	2045
1,3-Diphenyl-2-ethylpropane	Glass	314.6	1.5491	.96457	50.3	6.44	3.40	1.62	2190
1,3-Diphenyl-2-propylpropane	Glass	323.2	1.5424	.95352	70.8	7.43	3.75	1.71	2345
1,3-Dicyclohexyl-2-methylpropane	0.57	295.2	1.4756	.87151	35.8	7.12	4.02	1.99	2300
1,3-Dicyclohexyl-2-ethylpropane	Glass	306.1	1.4773	.87491	72.1	9.42	4.80	2.20	2445
1,3-Dicyclohexyl-2-propylpropane	Glass	316.1	1.4764	.87191	(d)	12.60	5.82	2.44	2590

[a]With slight decomposition.
[b]A.S.T.M. procedure: D445-46T.
[c]Equilibrium portion of melting curve was very short.
[d]Value obtained is omitted because it was at variance with the other values when plotted on A.S.T.M. standard viscosity-temperature chart, D341-chart E.

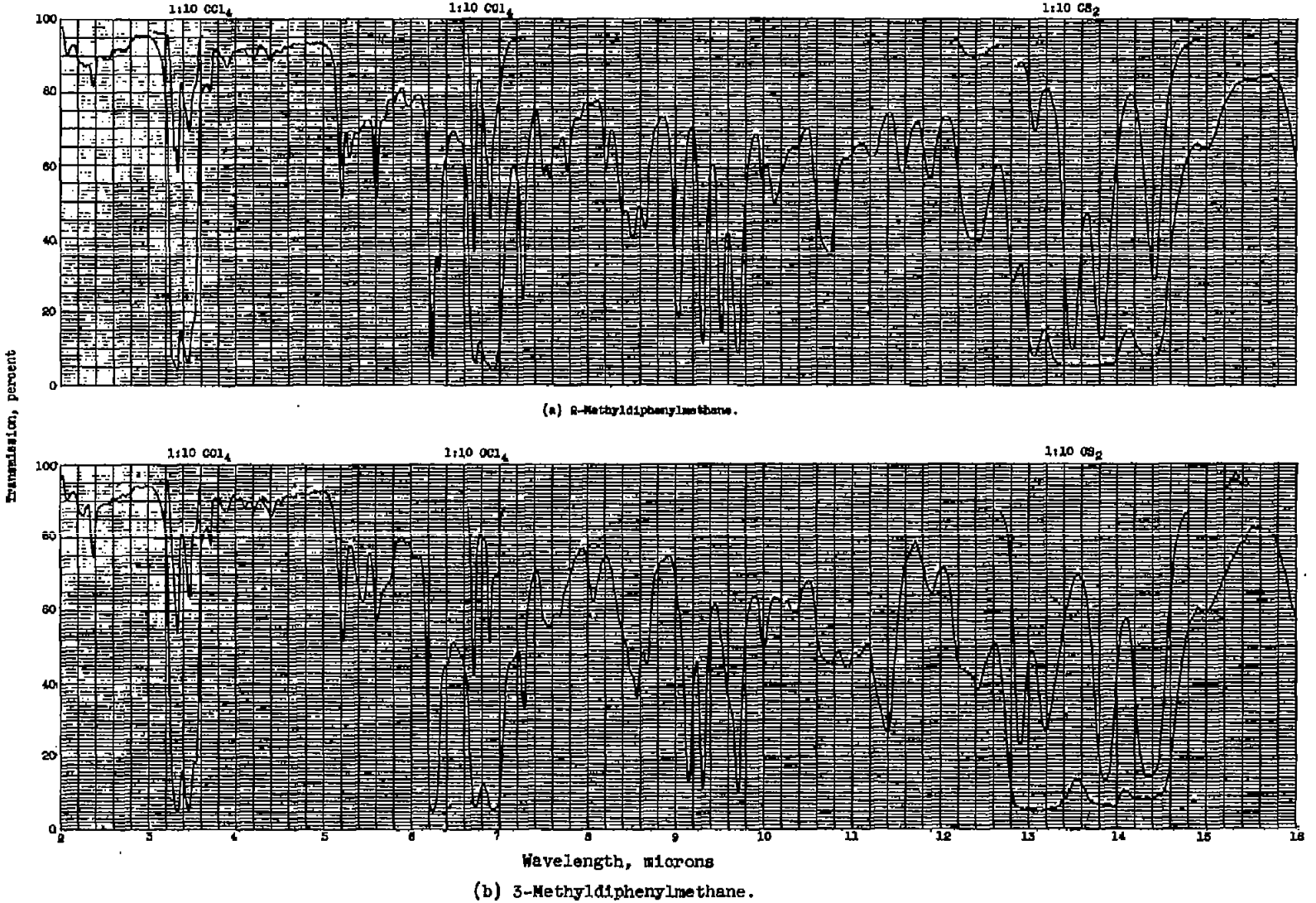
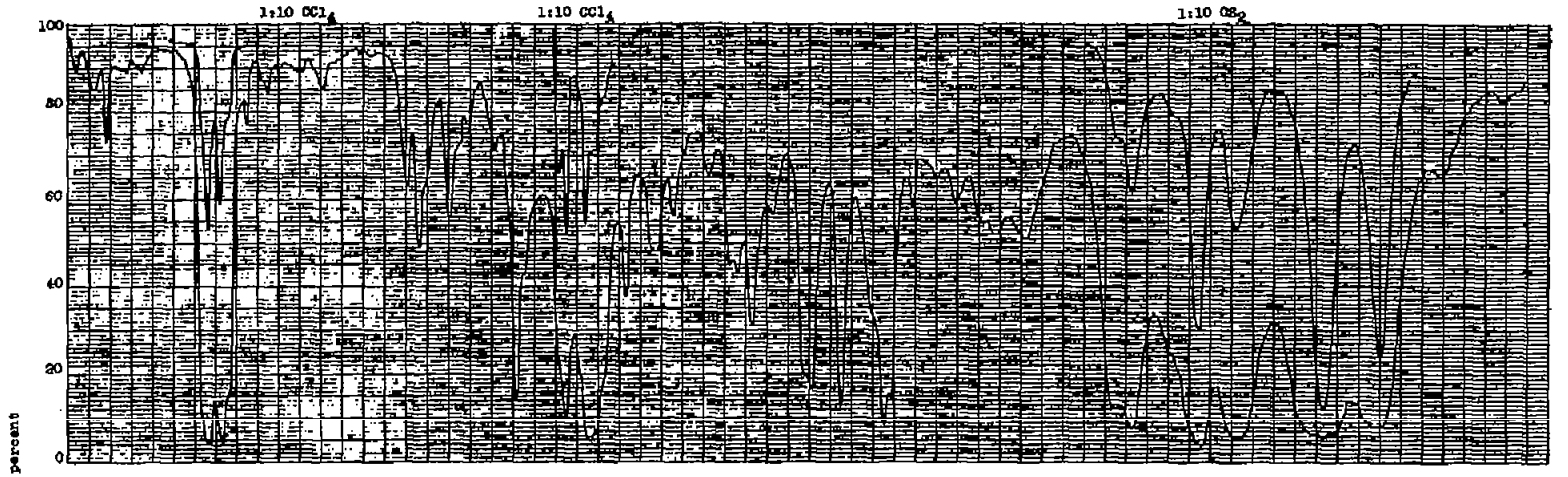
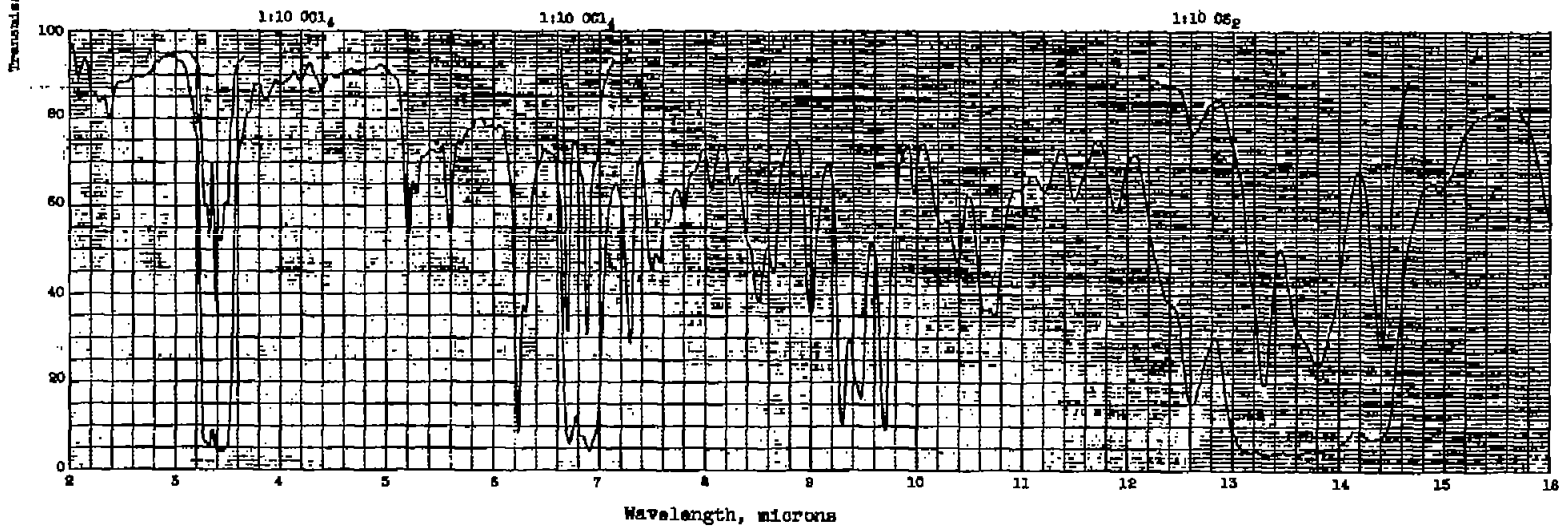


Figure 1. - Infrared spectra for alkyldiphenylmethanes. Cell width, 0.1 millimeter; sample undiluted or diluted as indicated.



(c) 4-Methyldiphenylmethane.



(d) 2-Ethyldiphenylmethane.

Figure 1. - Continued. Infrared spectra for alkyldiphenylmethanes. Cell width, 0.1 millimeter; sample undiluted or diluted as indicated.

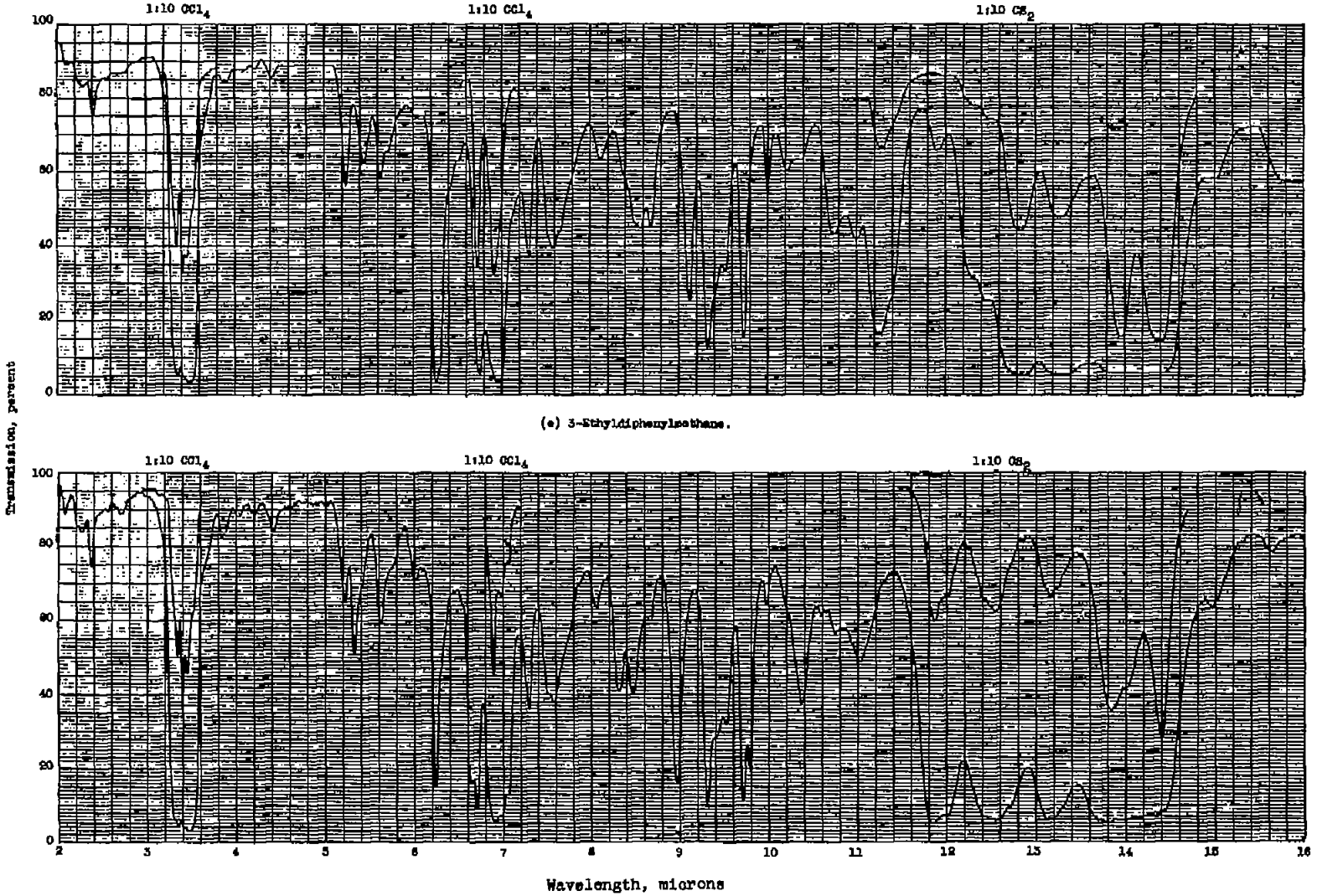
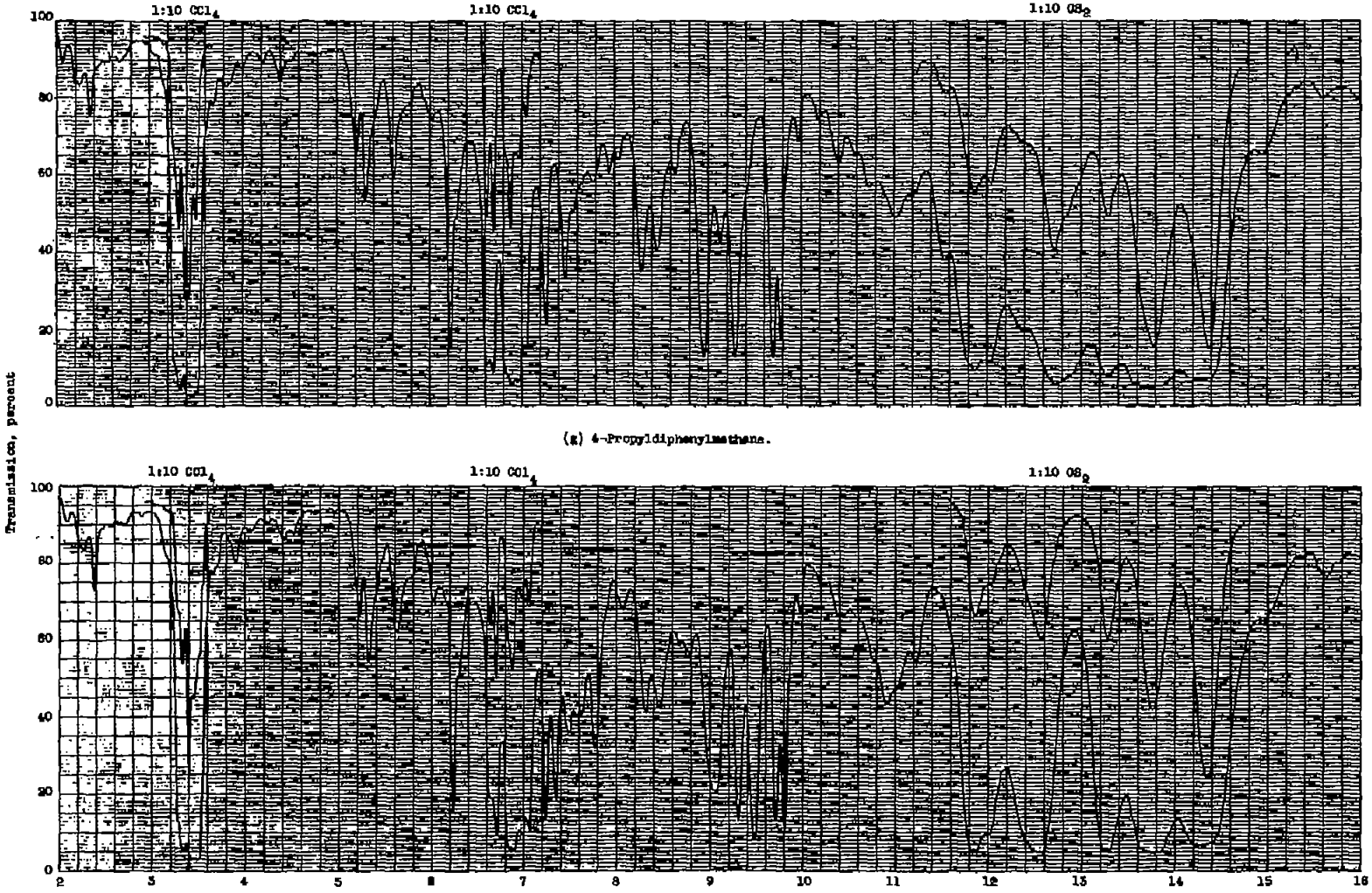


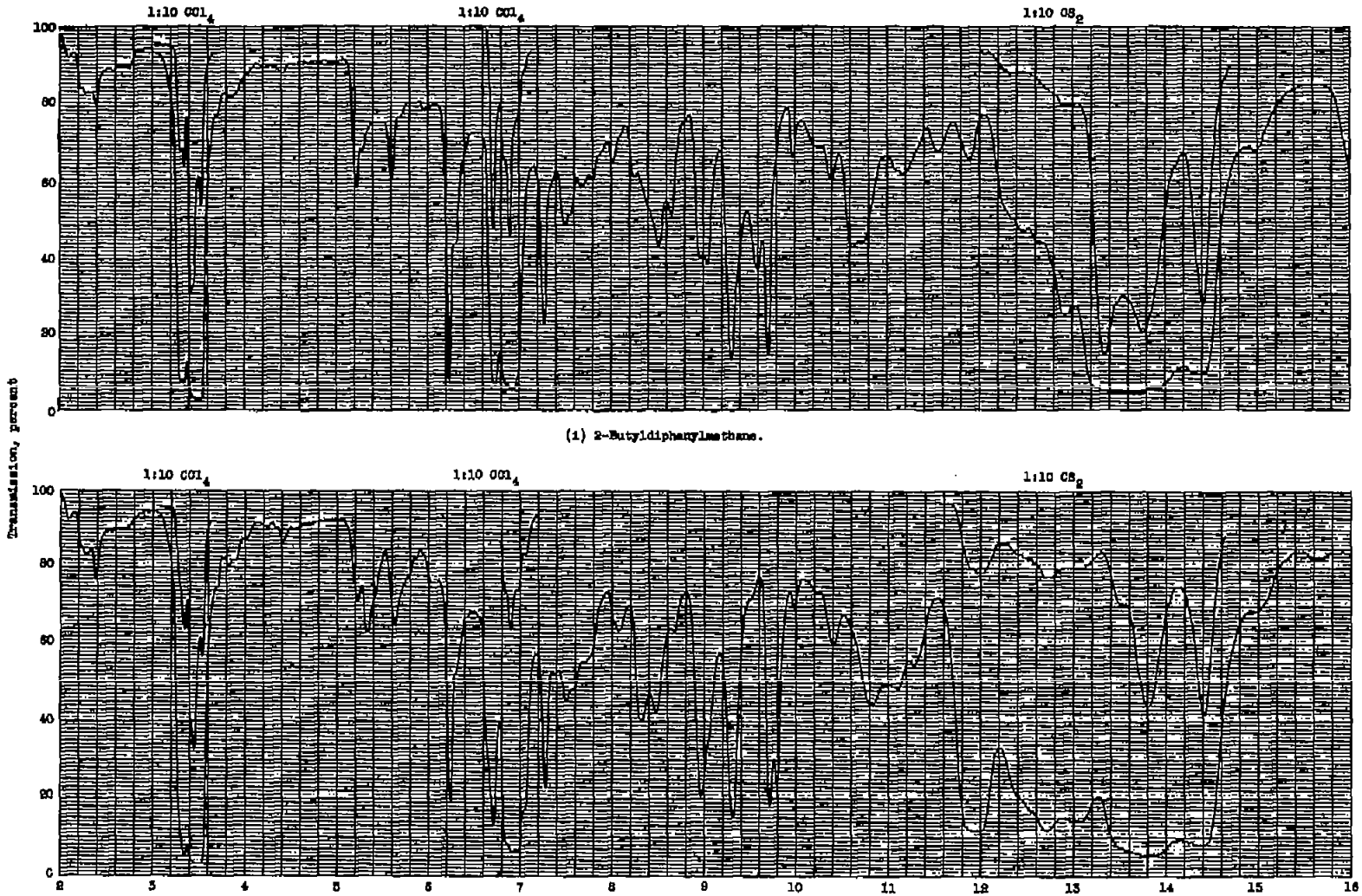
Figure 1. - Continued. Infrared spectra for alkyldiphenylmethanes. Cell width, 0.1 millimeter; sample undiluted or diluted as indicated.



(g) 4-Propyldiphenylmethane.

(h) 4-Isopropyldiphenylmethane.

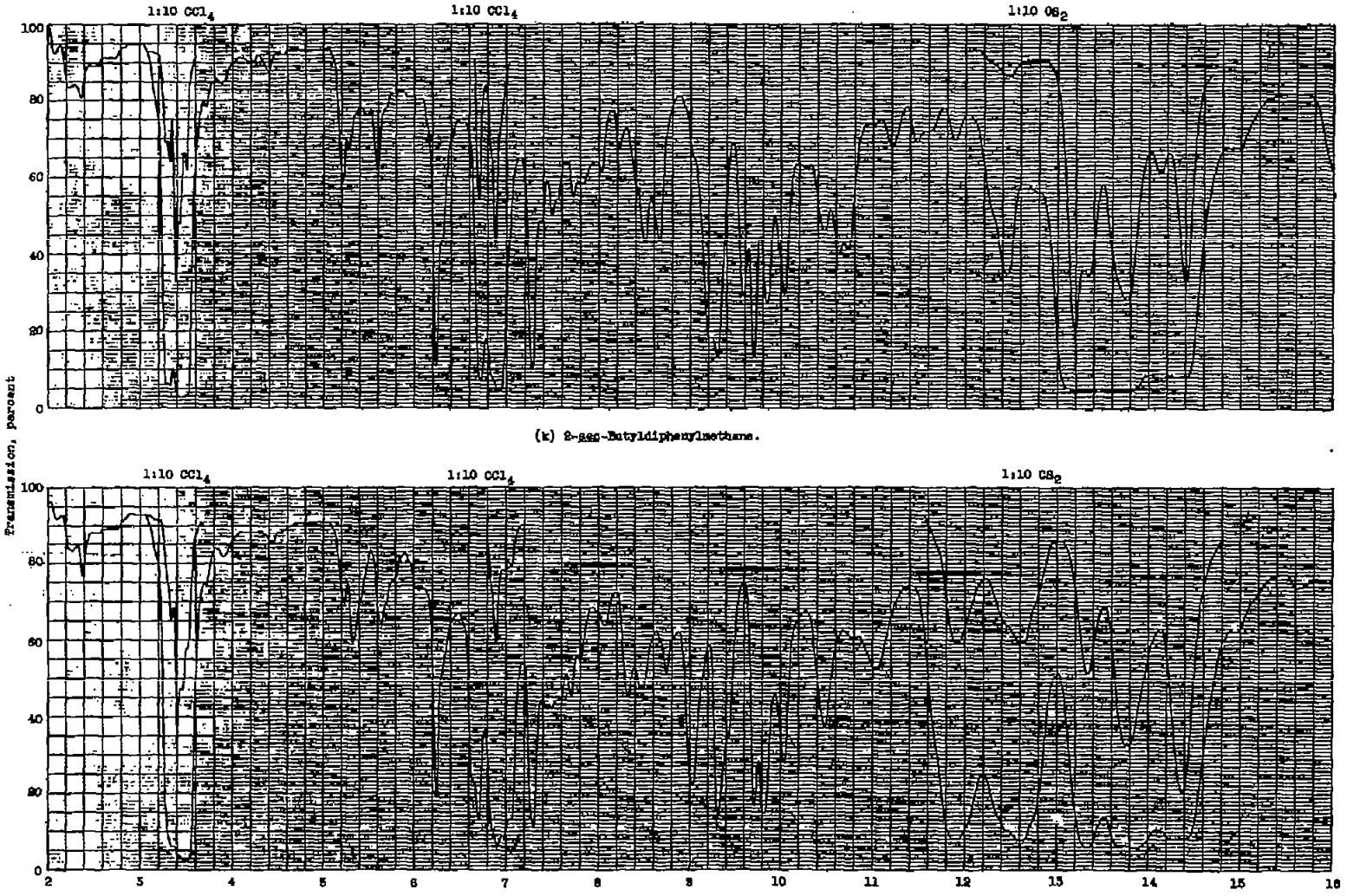
Figure 1. - Continued. Infrared spectra for alkyldiphenylmethanes. Cell width, 0.1 millimeter; sample undiluted or diluted as indicated.



(i) 2-Butyldiphenylmethane.

(j) 4-Butyldiphenylmethane.

Figure 1. - Continued. Infrared spectra for alkyldiphenylmethanes. Cell width, 0.1 millimeter; sample undiluted or diluted as indicated.



(k) 2-sec-Butyldiphenylmethane.

(l) 4-sec-Butyldiphenylmethane.

Figure 1. - Concluded. Infrared spectra for alkyldiphenylmethanes. Cell width, 0.1 millimeter; sample undiluted or diluted as indicated.

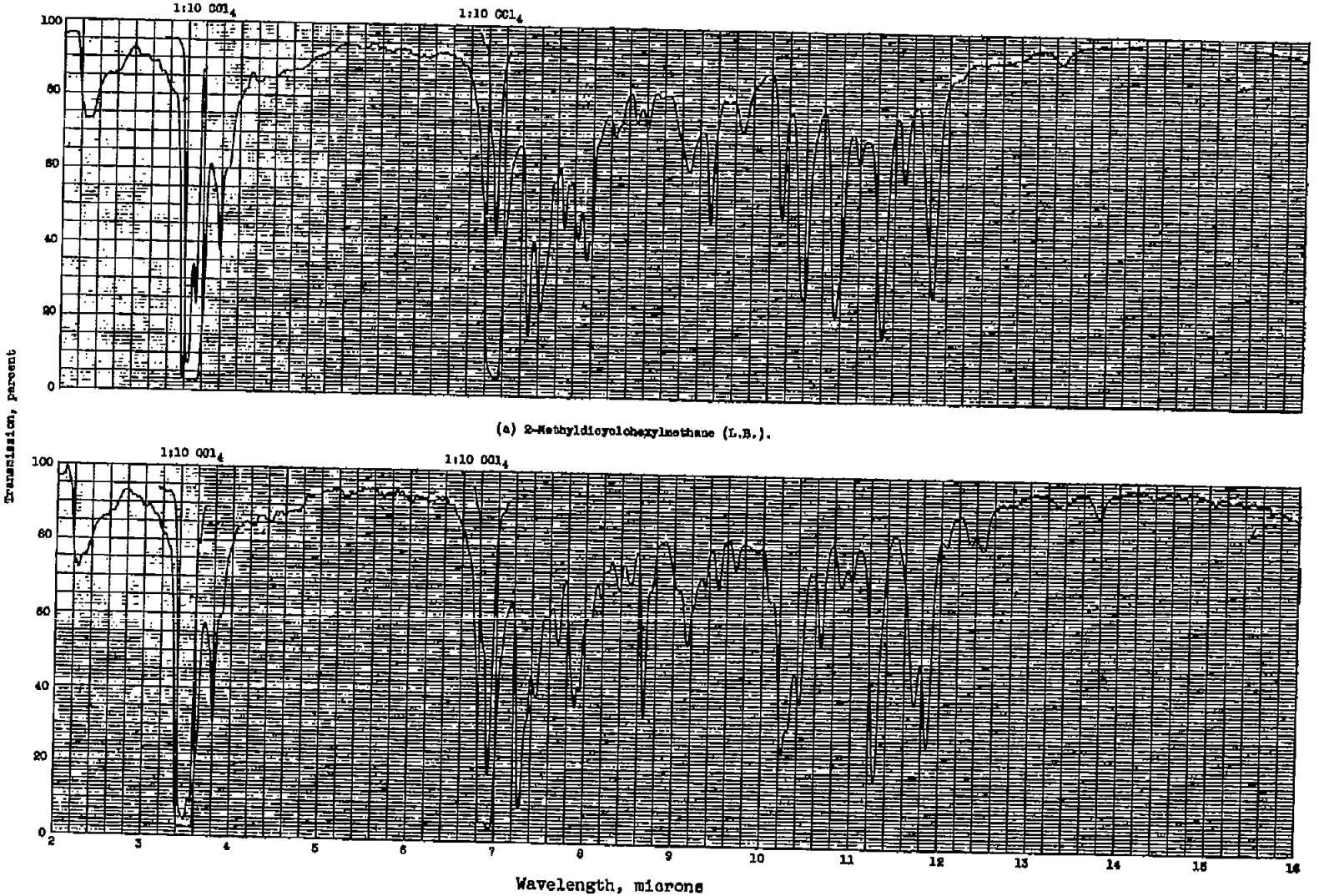


Figure 2. - Infrared spectra for alkyldicyclohexylmethanes. Cell width, 0.1 millimeter; sample undiluted or diluted as indicated.

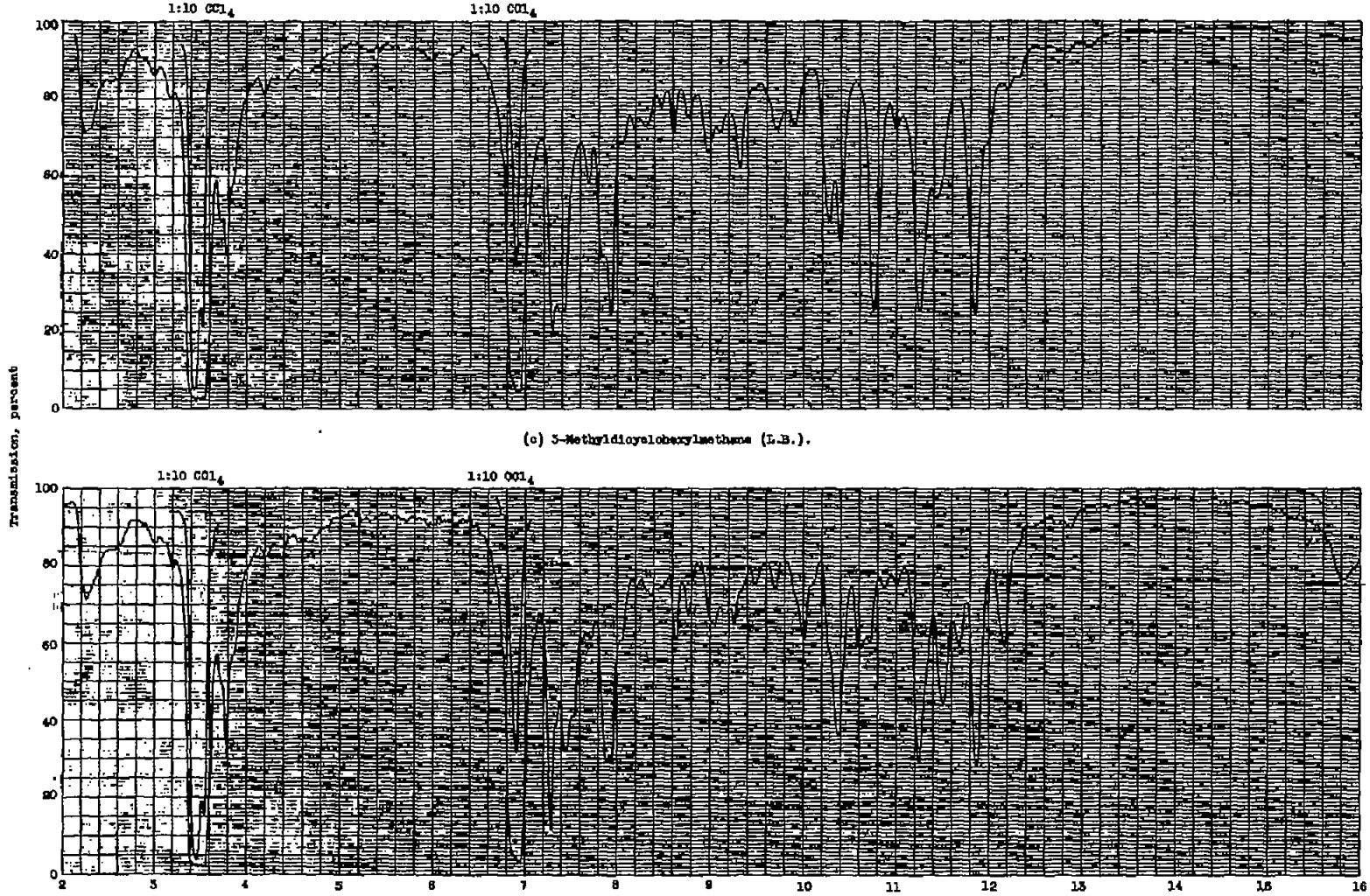


Figure 2. - Continued. Infrared spectra for alkyldicyclohexylmethanes. Cell width, 0.1 millimeter; sample undiluted or diluted as indicated.

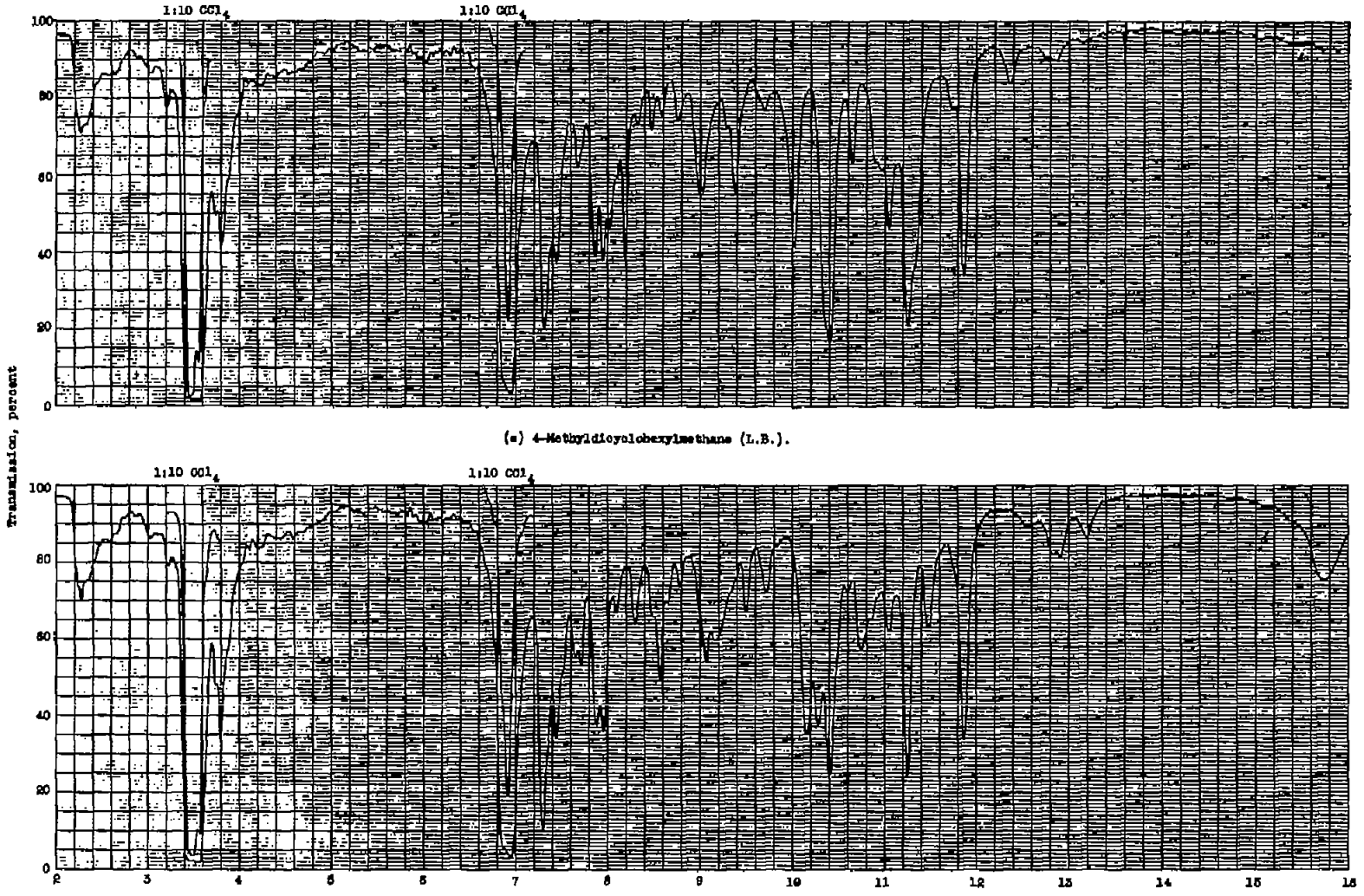
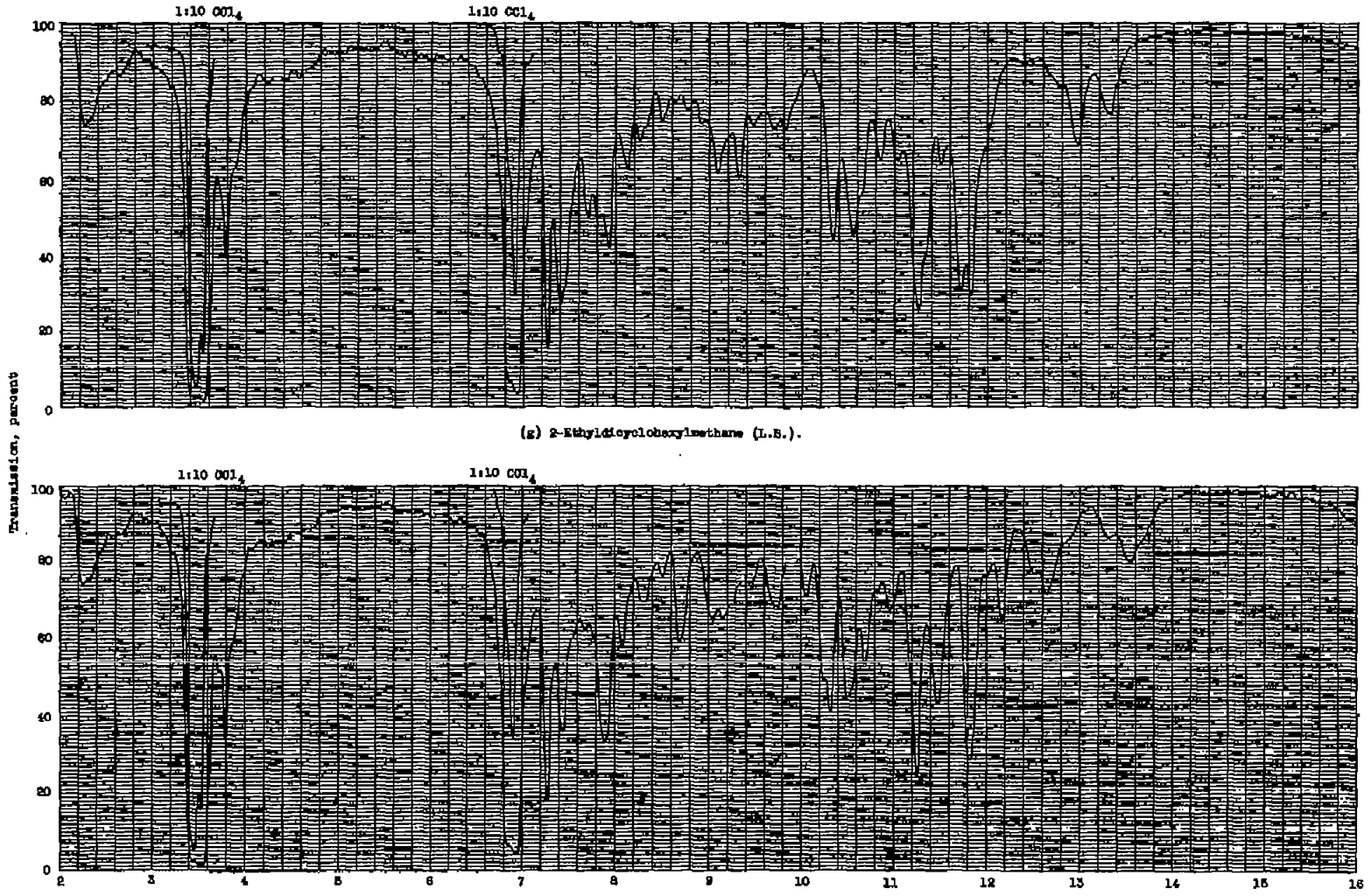


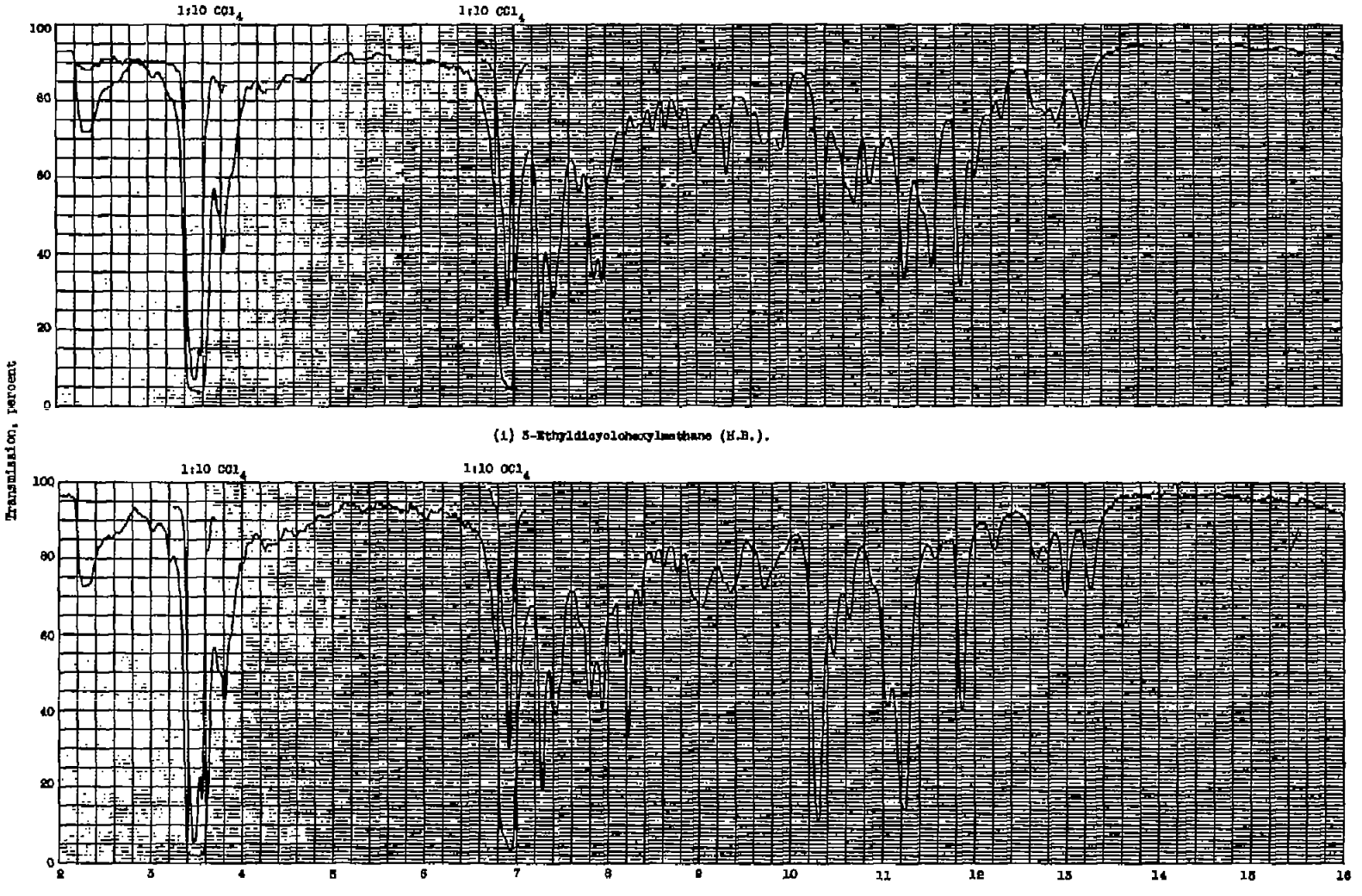
Figure 2. - Continued. Infrared spectra for alkyldicyclohexylmethanes. Cell width, 0.1 millimeter; sample undiluted or diluted as indicated.



(g) 2-Ethyldicyclohexylmethane (L.S.).

(h) 2-Ethyldicyclohexylmethane (H.B.).

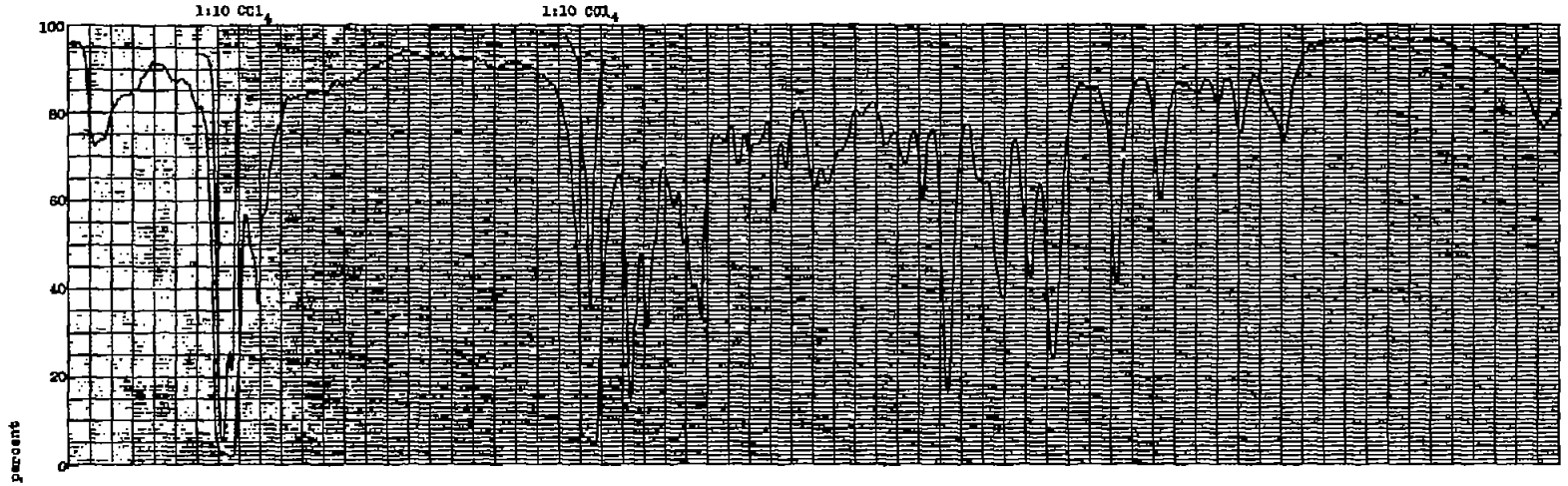
Figure 2. - Continued. Infrared spectra for alkyldicyclohexylmethanes. Cell width, 0.1 millimeter; sample undiluted or diluted as indicated.



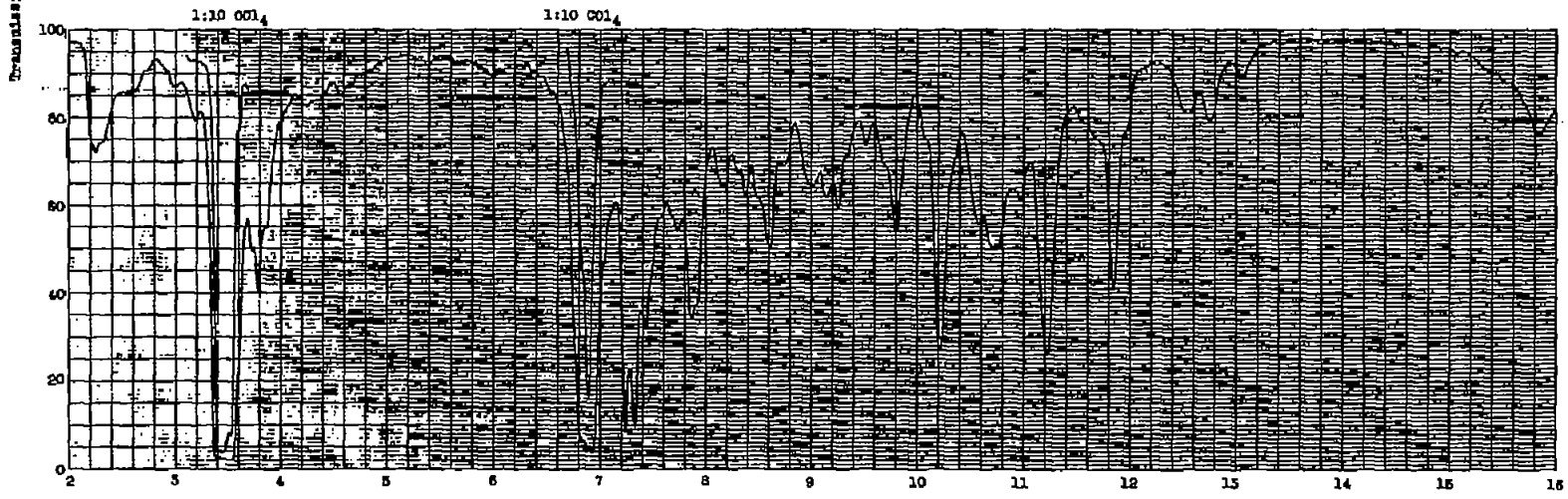
(i) 5-Ethyldicyclohexylmethane (H.B.).

(j) 4-Ethyldicyclohexylmethane (L.B.).

Figure 2. - Continued. Infrared spectra for alkyldicyclohexylmethanes. Cell width, 0.1 millimeter; sample undiluted or diluted as indicated.

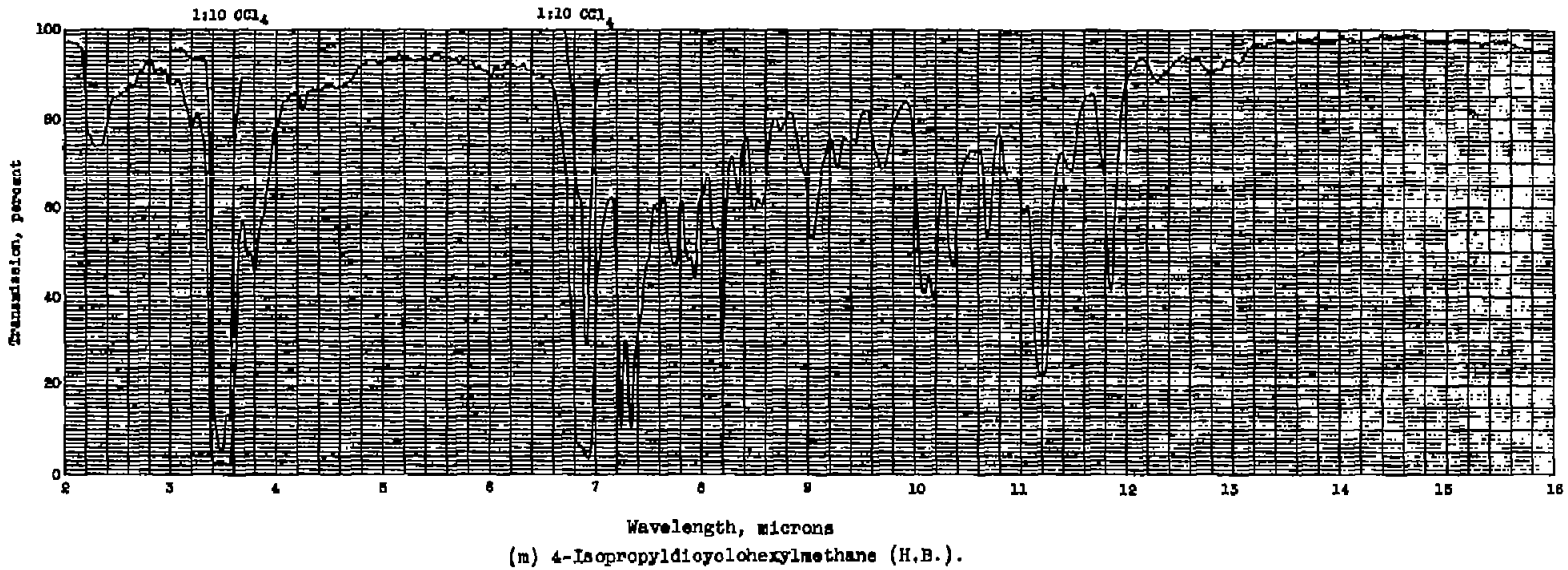


(k) 4-Ethyldicyclohexylmethane (H.B.).



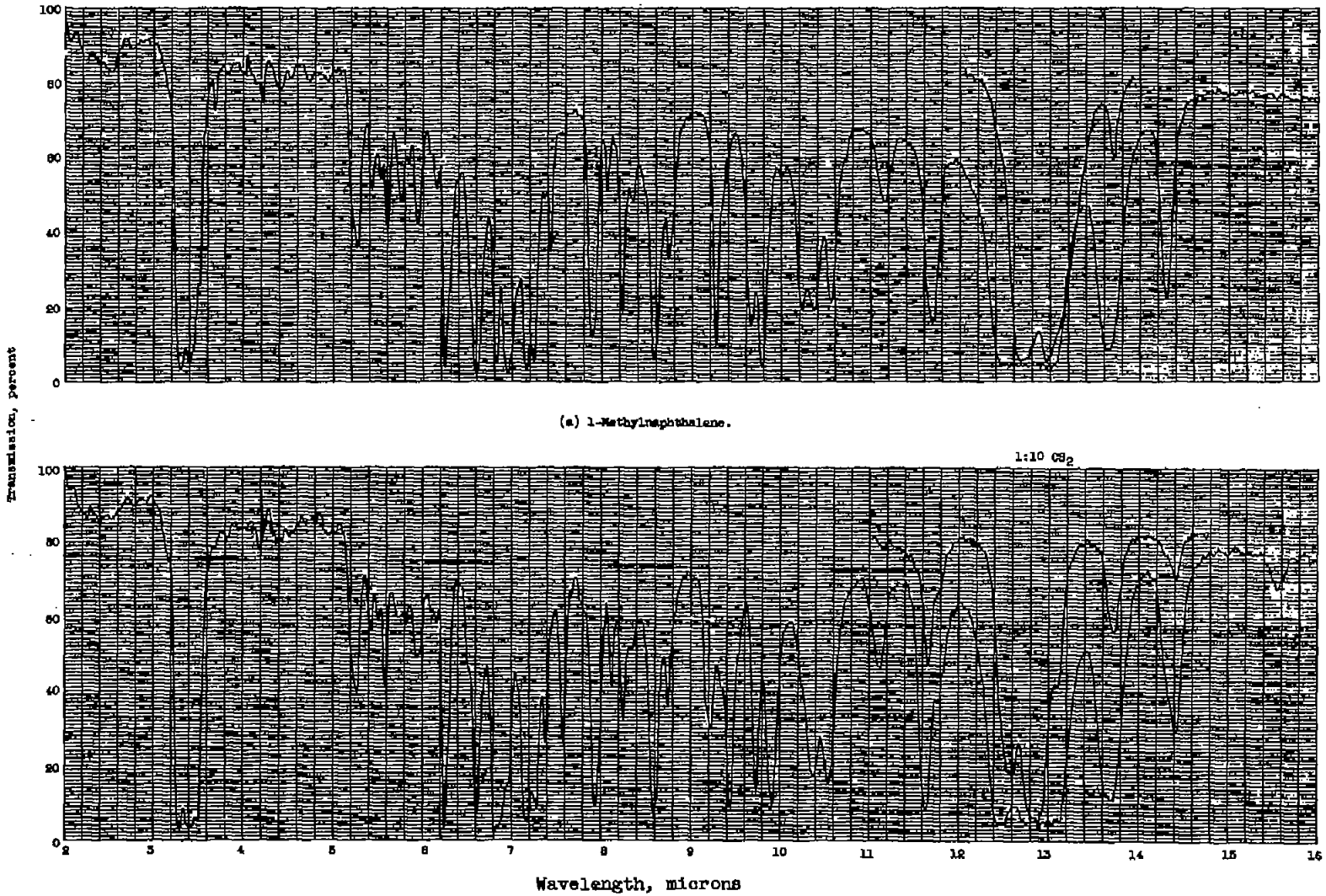
(l) 4-Isopropyldicyclohexylmethane (L.B.).

Figure 2. - Continued. Infrared spectra for alkyldicyclohexylmethanes. Cell width, 0.1 millimeter; sample undiluted or diluted as indicated.



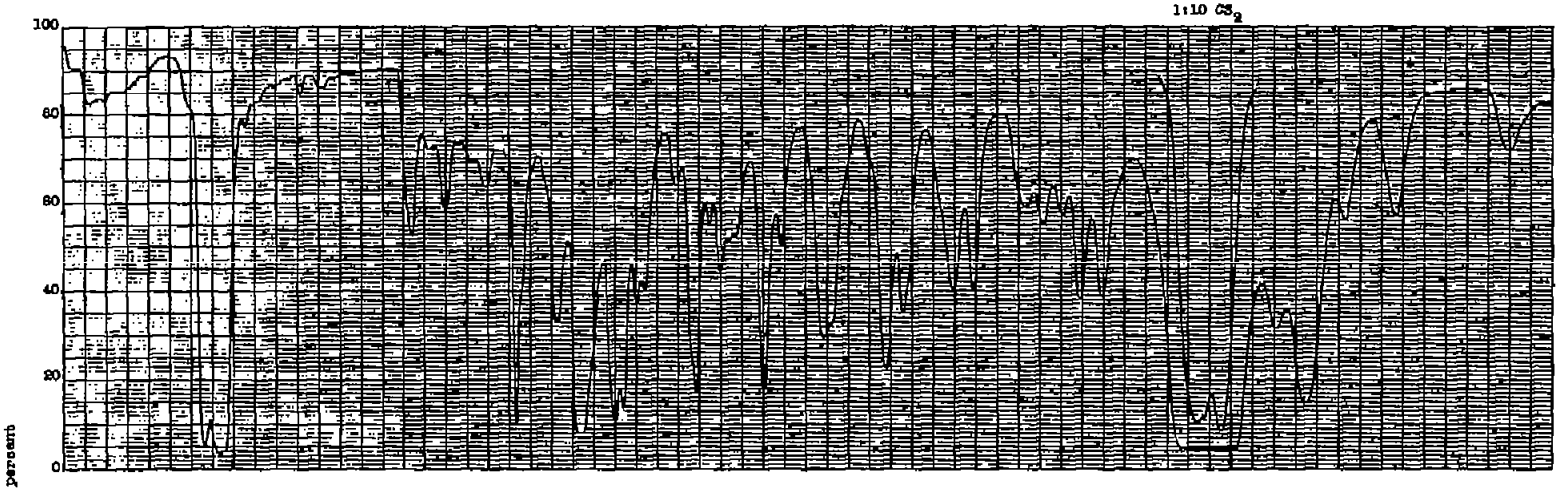
(m) 4-Isopropyldicyclohexylmethane (H.B.).

Figure 2. - Concluded. Infrared spectra for alkyldicyclohexylmethanes. Cell width, 0.1 millimeter; sample undiluted or diluted as indicated.

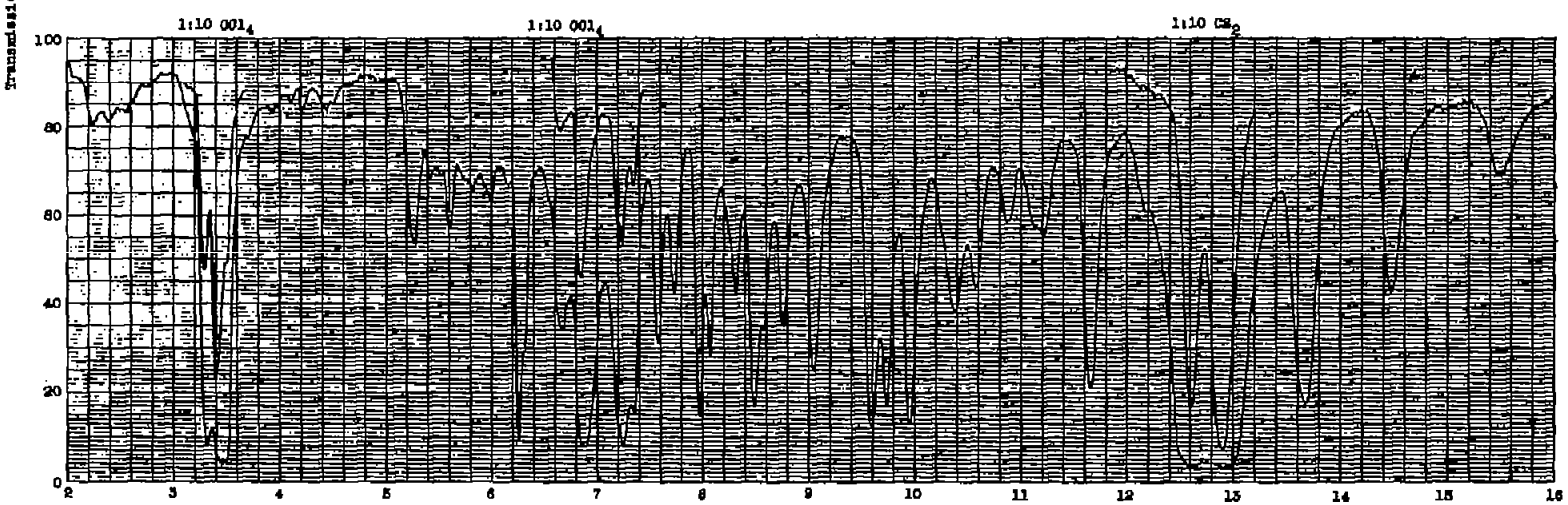


(b) 1-Ethylnaphthalene.

Figure 3. - Infrared spectra for alkylnaphthalenes. Cell width, 0.1 millimeter; sample undiluted or diluted as indicated.

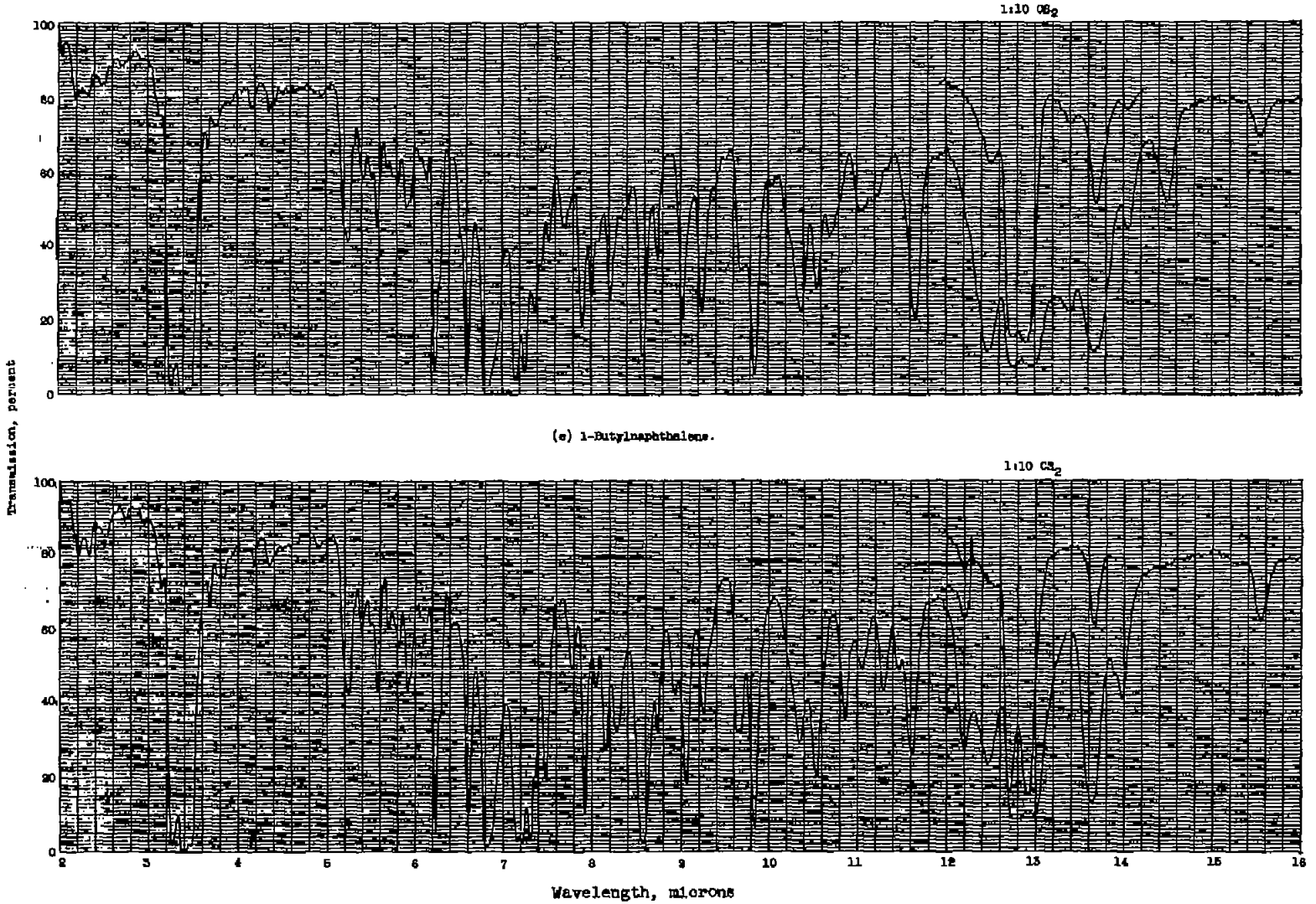


(c) 1-Propylnaphthalene.



(d) 1-Isopropylnaphthalene.

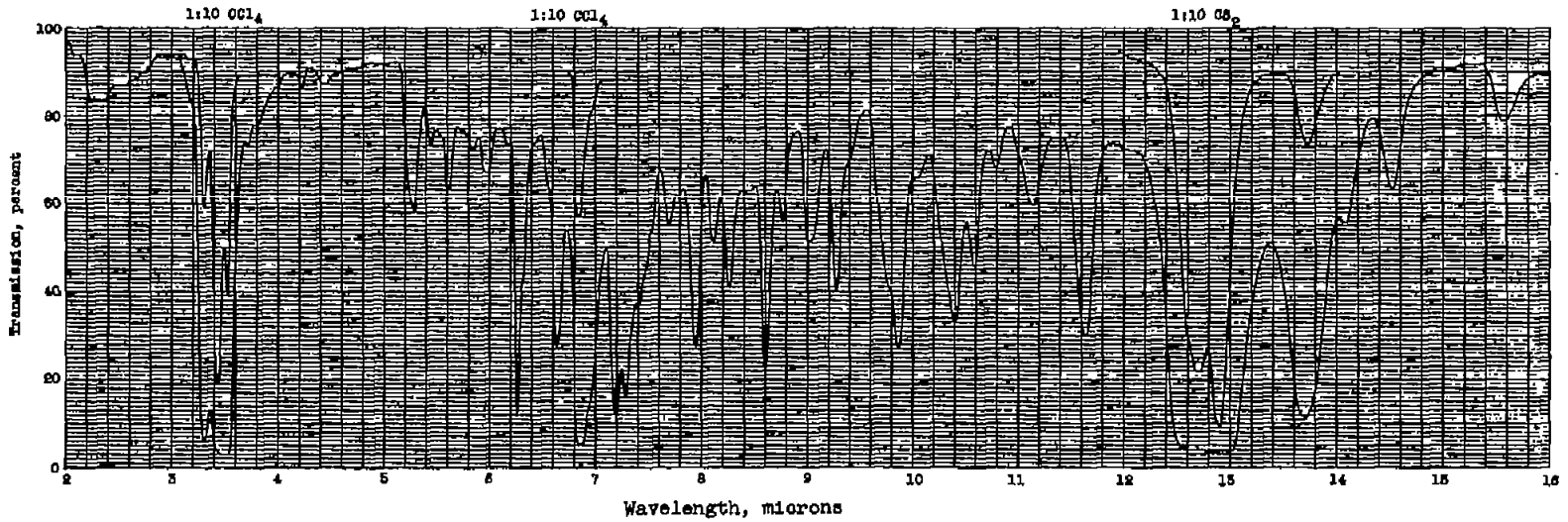
Figure 3. - Continued. Infrared spectra for alkylnaphthalenes. Cell width, 0.1 millimeter; sample undiluted or diluted as indicated.



(e) 1-Butylnaphthalene.

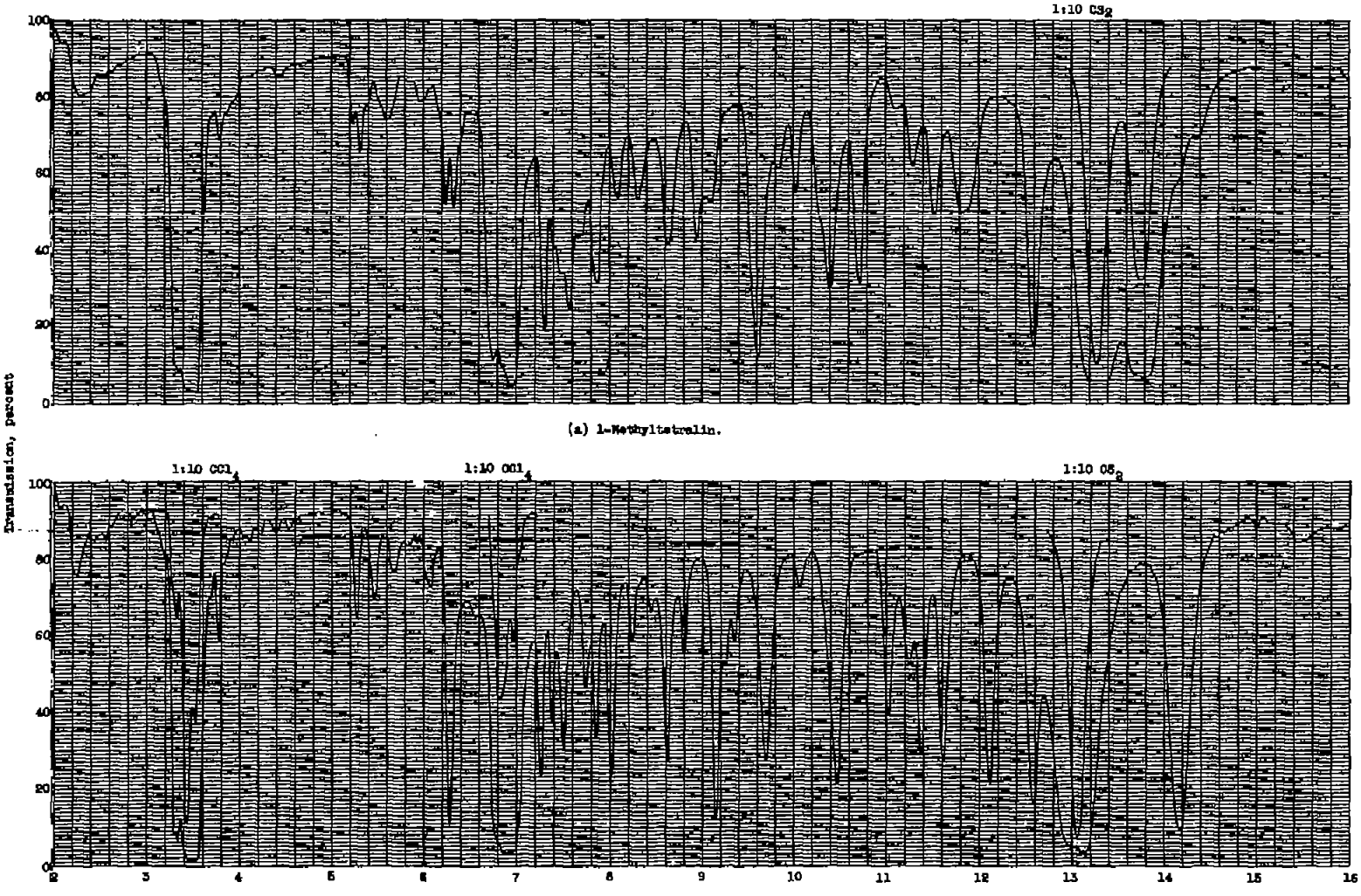
(f) 1-Isobutylnaphthalene.

Figure 3. - Continued. Infrared spectra for alkylnaphthalenes. Cell width, 0.1 millimeter; sample undiluted or diluted as indicated.



(g) 1- Amylnaphthalene.

Figure 3. - Concluded. Infrared spectra for alkylnaphthalenes. Cell width, 0.1 millimeter; sample undiluted or diluted as indicated.



(b) 5-Methyltetralin.

Figure 4. - Infrared spectra for alkyltetralins. Cell width, 0.1 millimeter; sample undiluted or diluted as indicated.

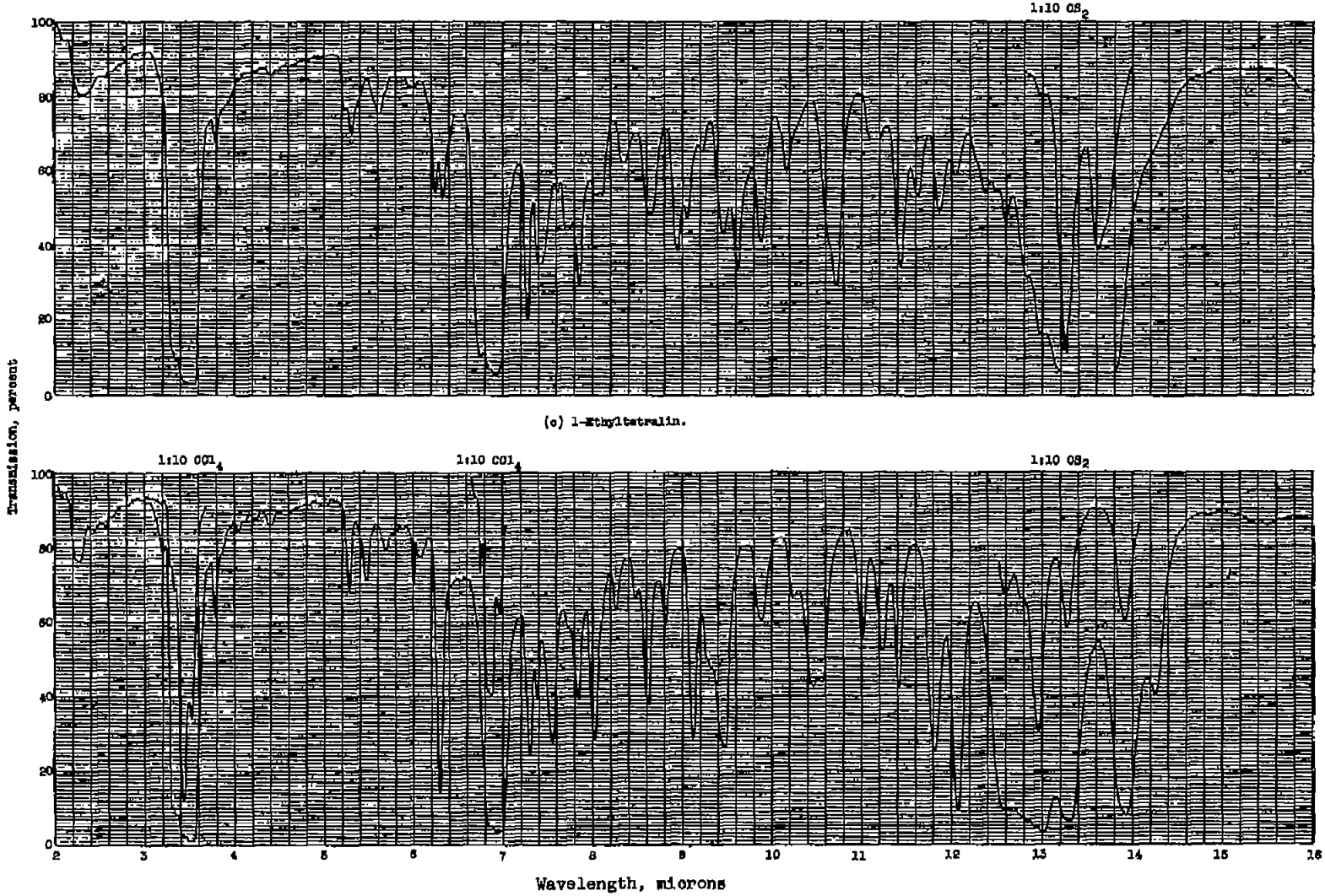


Figure 4. - Continued. Infrared spectra for alkyltetralins. Cell width, 0.1 millimeter; sample undiluted or diluted as indicated.

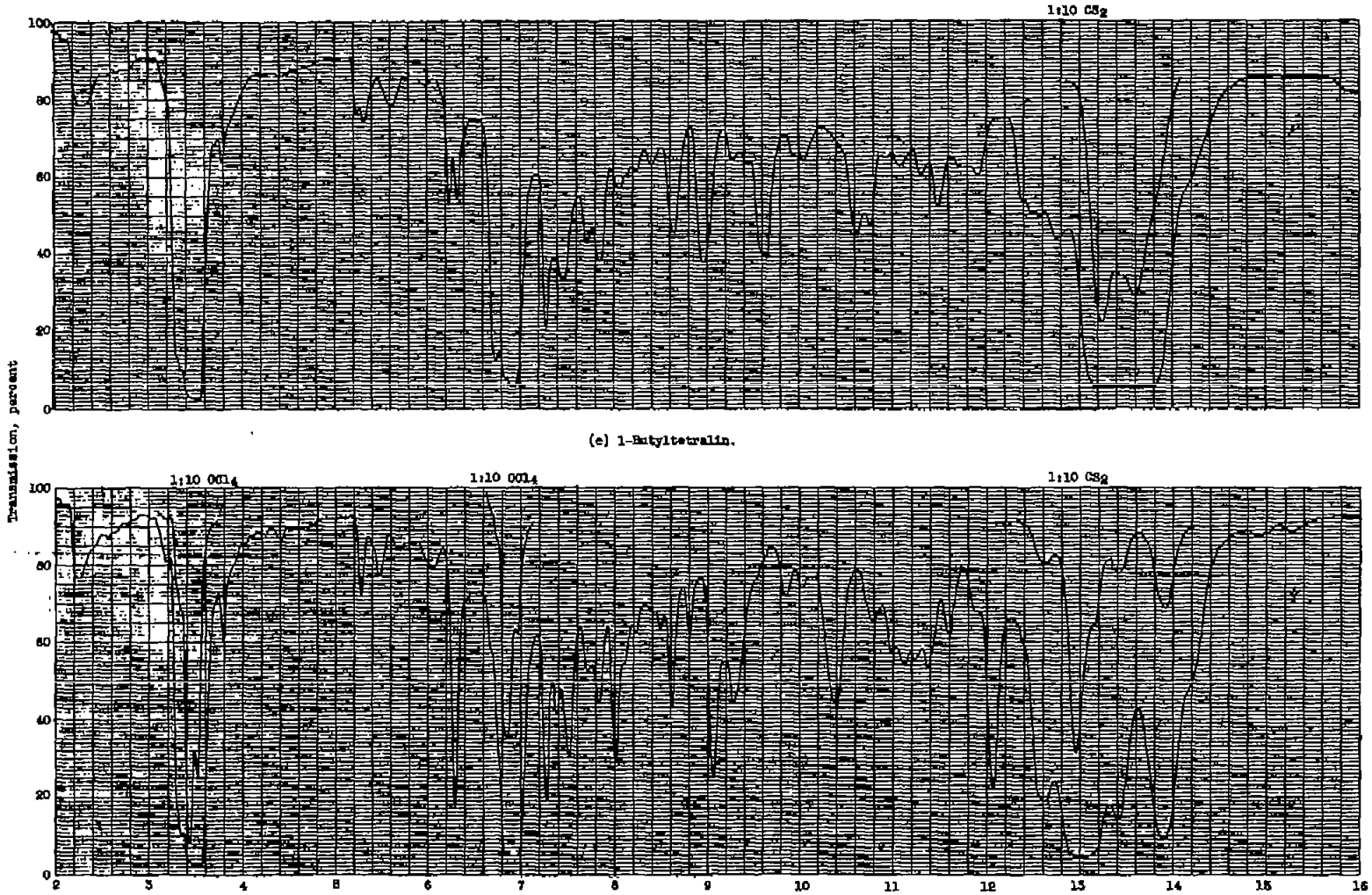
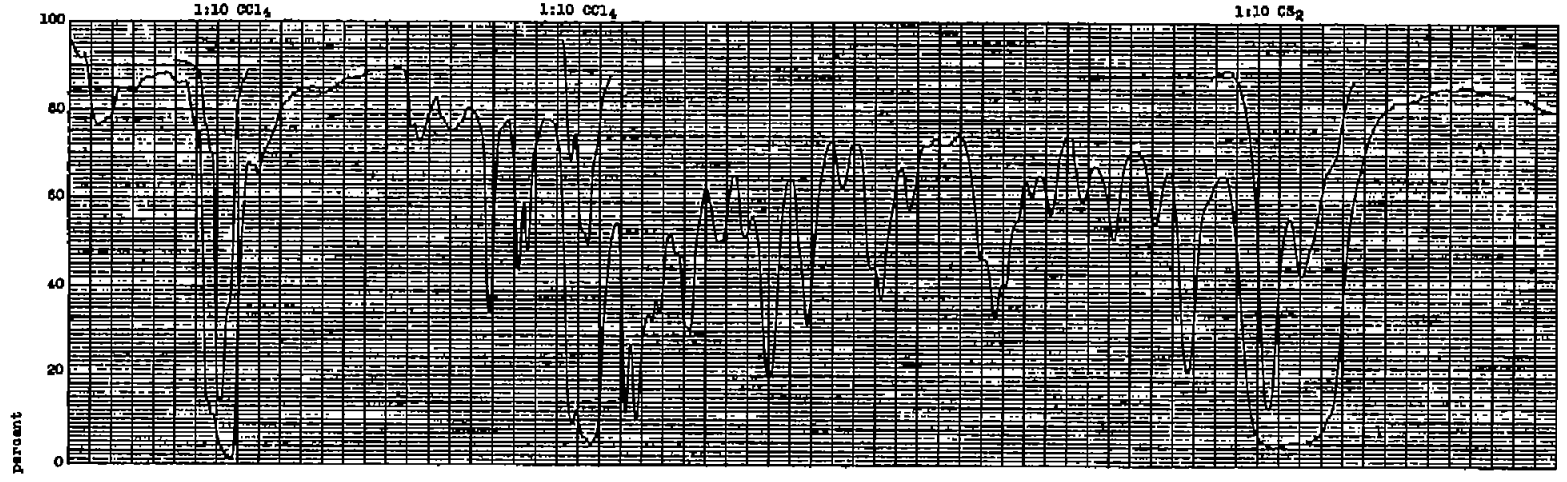
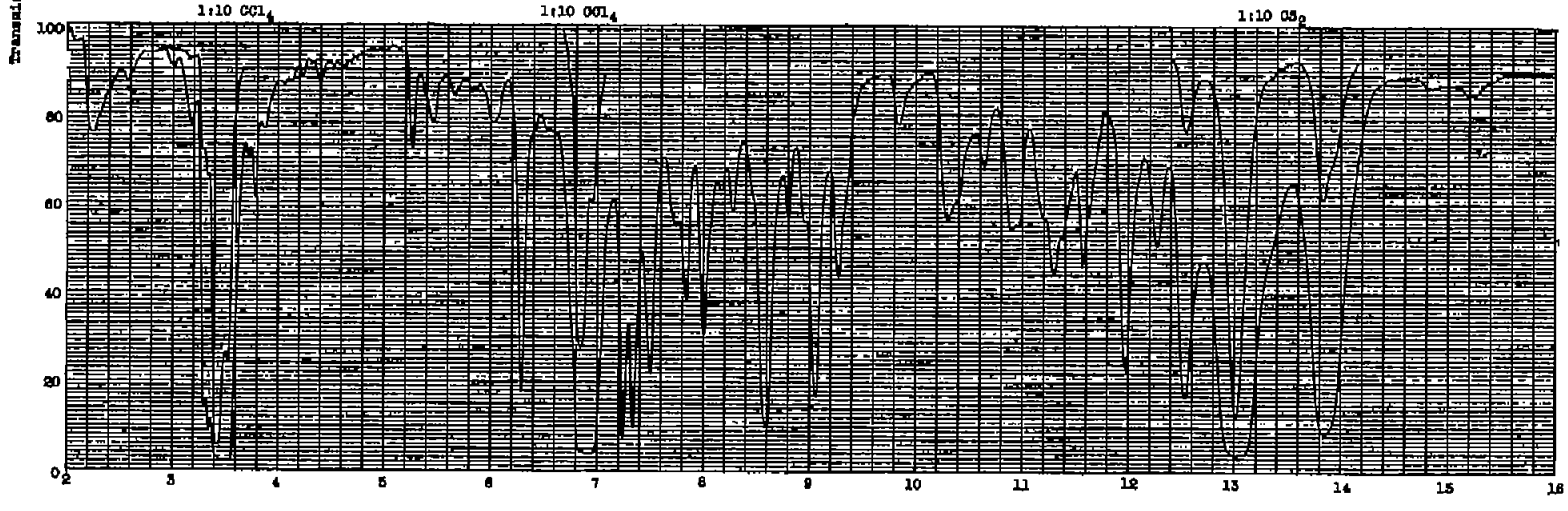


Figure 4. - Continued. Infrared spectra for alkyltetralins. Cell width, 0.1 millimeter; sample undiluted or diluted as indicated.



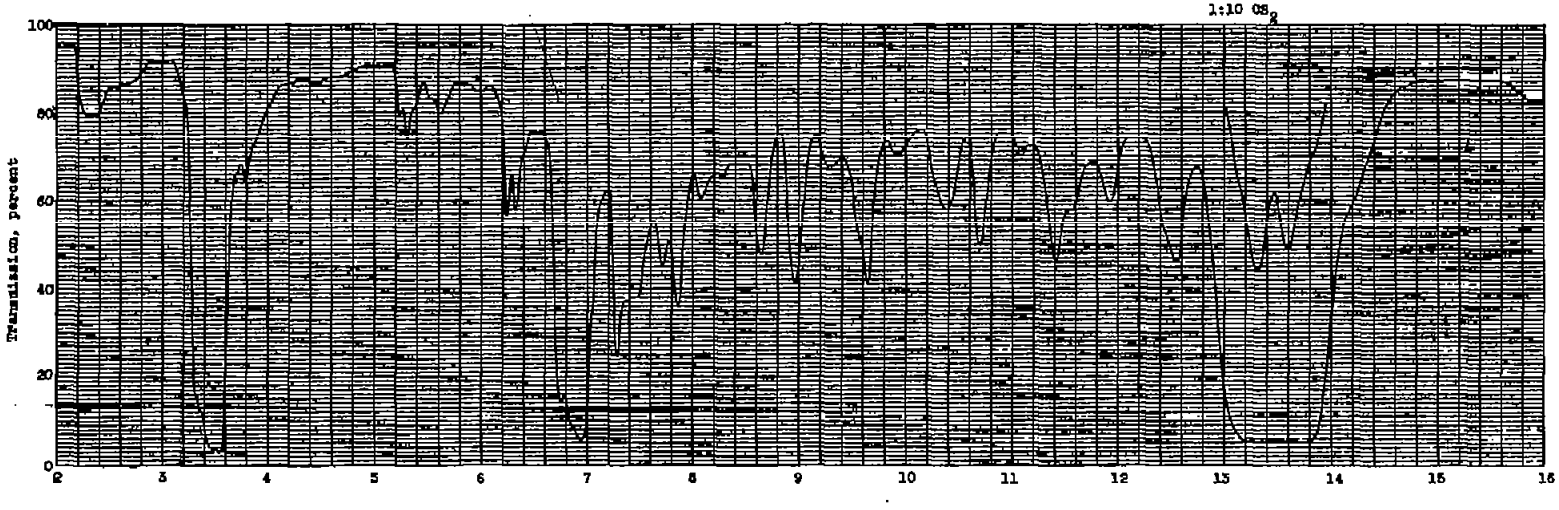
(g) 1-Isobutyltetralin.



Wavelength, microns

(h) 5-Isobutyltetralin.

Figure 4. - Continued. Infrared spectra for alkyltetralins. Cell width, 0.1 millimeter; sample undiluted or diluted as indicated.



(i) 1-Amyltetralin.

Figure 4. - Concluded. Infrared spectra for alkyltetralins. Cell width, 0.1 millimeter; sample undiluted or diluted as indicated.

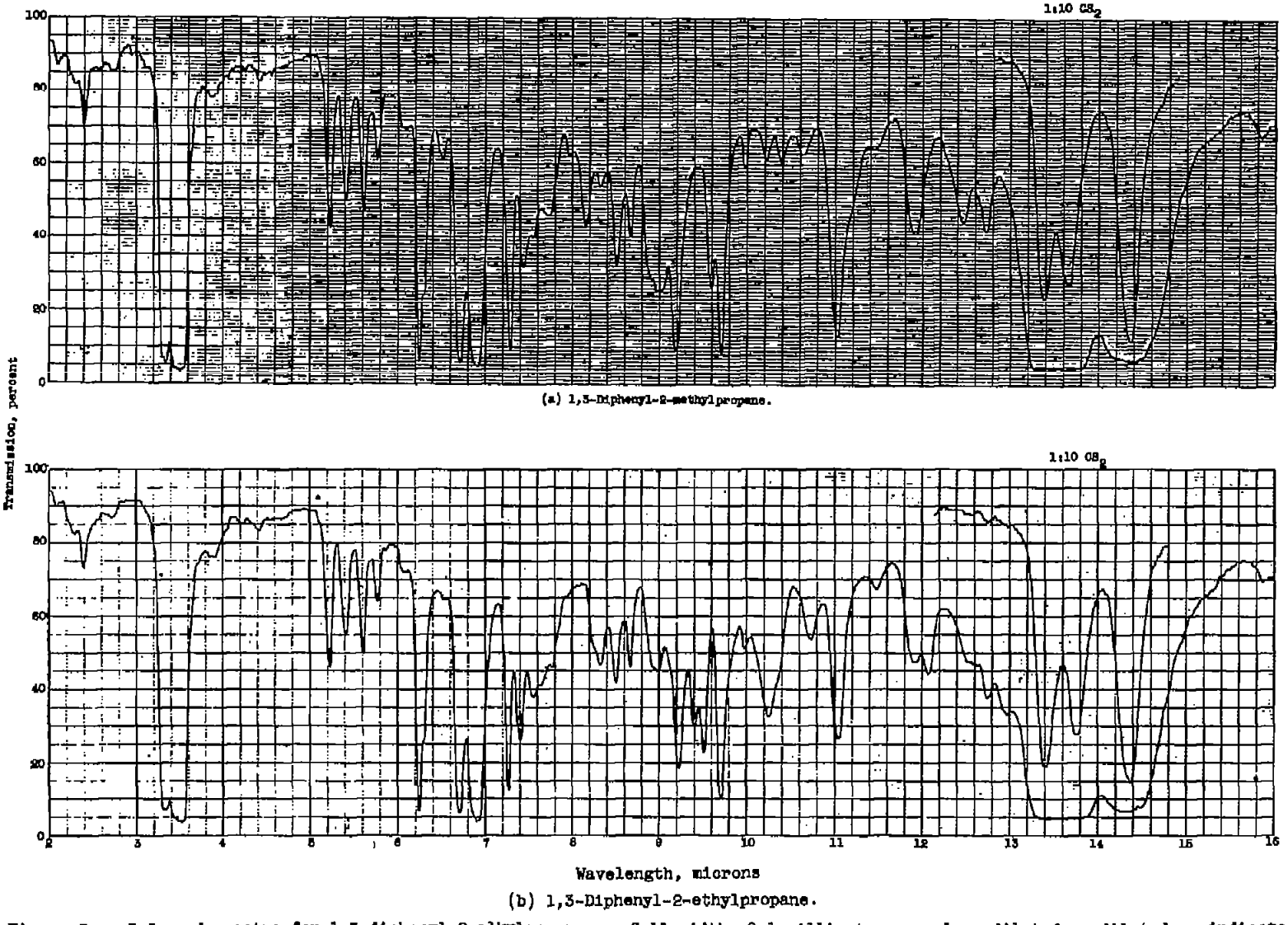
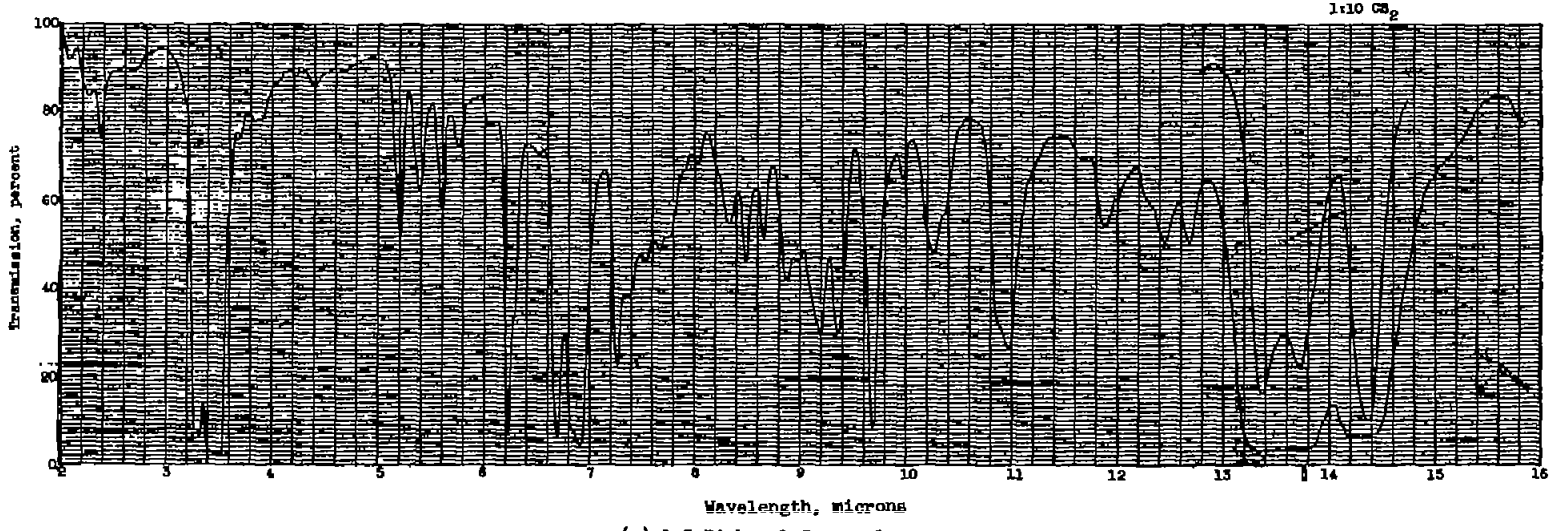
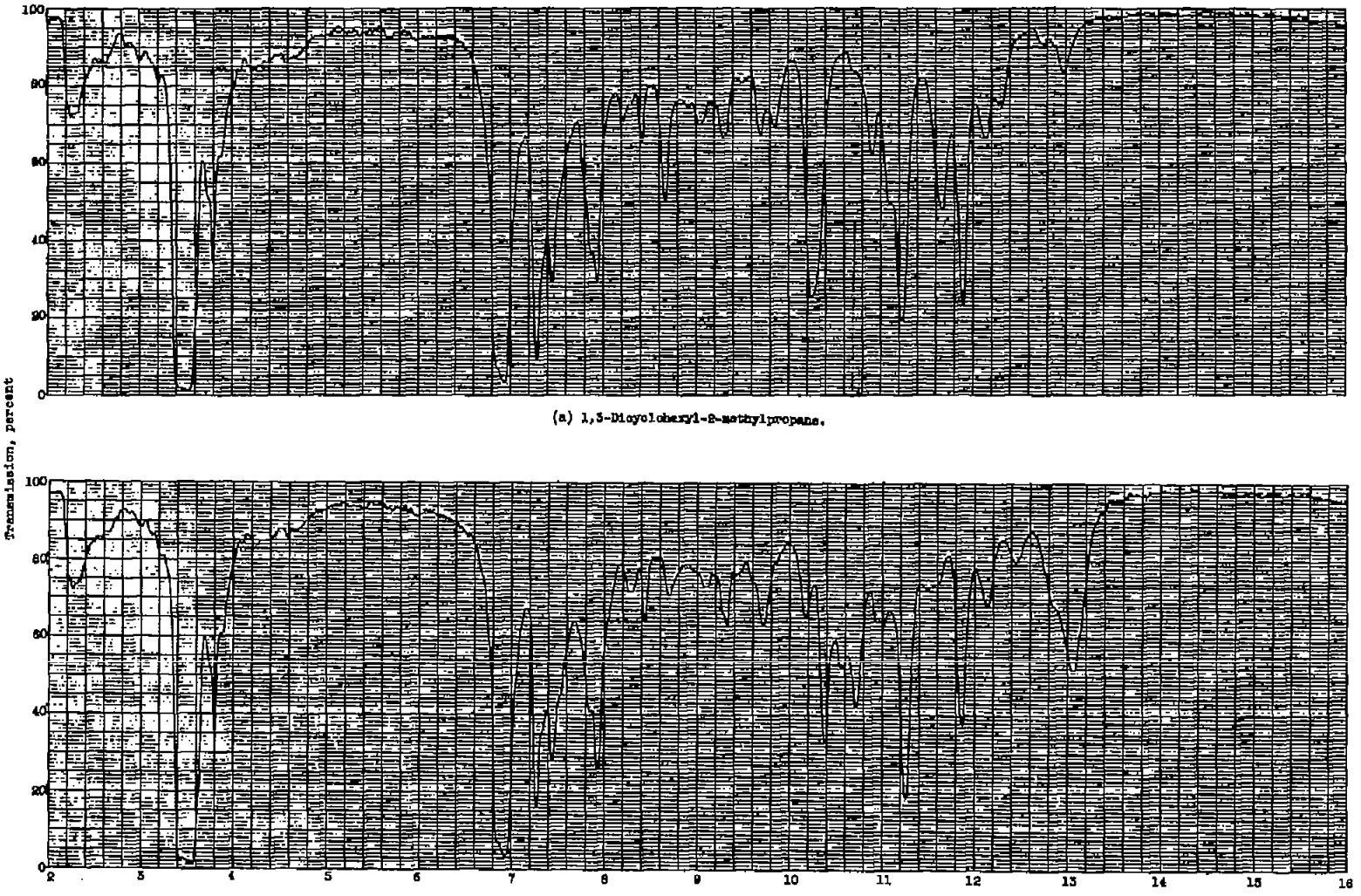


Figure 5. - Infrared spectra for 1,3-diphenyl-2-alkylpropanes. Cell width, 0.1 millimeter; sample undiluted or diluted as indicated.



(a) 1,3-Diphenyl-2-propylpropane.

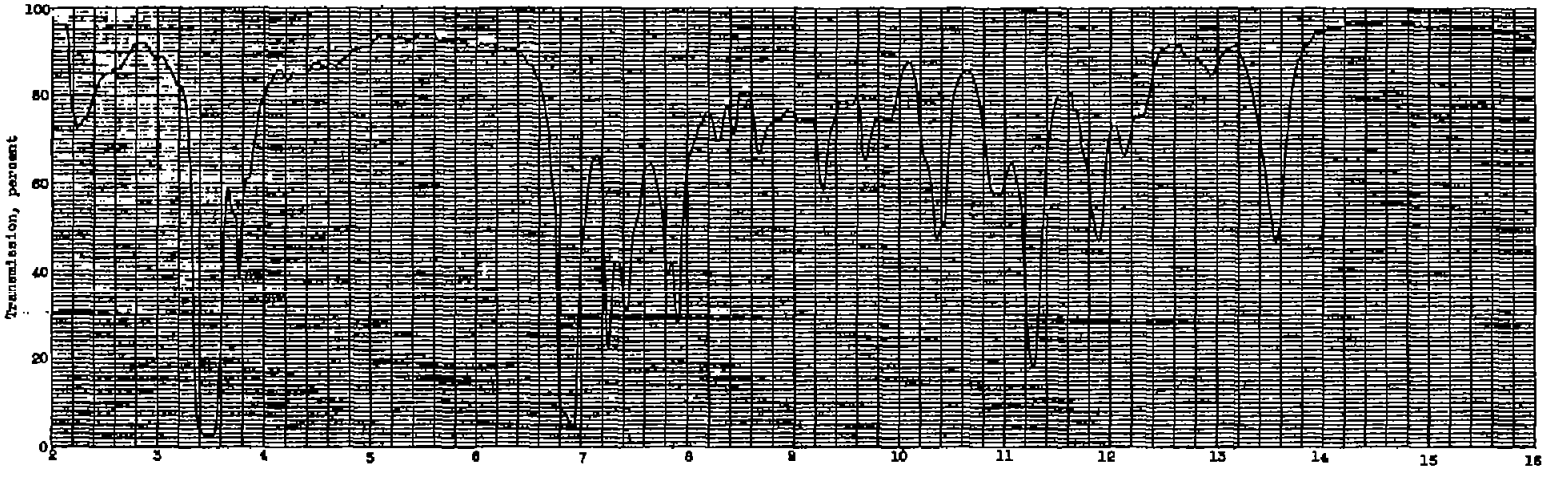
Figure 5. - Concluded. Infrared spectra for 1,3-diphenyl-2-alkylpropanes. Cell width, 0.1 millimeter; sample undiluted or diluted as indicated.



(a) 1,3-Dicyclohexyl-2-methylpropane.

(b) 1,3-Dicyclohexyl-2-ethylpropane.

Figure 6. - Infrared spectra for 1,3-dicyclohexyl-2-alkylpropanes. Cell width, 0.1 millimeter; sample undiluted.



(c) 1,3-Dicyclohexyl-2-propylpropane.

Figure 6. - Concluded. Infrared spectra for 1,3-dicyclohexyl-2-alkylpropanes. Cell width, 0.1 millimeter; sample undiluted.

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